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This volume 1) discusses models which identify source contributions to receptor concentrations, their input data, the assumptions on which they are based, and the effects of typical deviations from those assumptions; 2) identifies measurements which these models require, their availability, the additional assumptions imposed by these measurements, and the effect of their precision and accuracy on modeling results; and 3)presents approaches, pertaining to three levels of analysis detail, for the optimum combinations of models and measurements in practical situations, and illustrates these protocols with case studies.

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Source Apportionment Techniques And Considerations In Combining Their Use

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PREFACE

Receptor Model Technical Series

Volume V

Source Apportionment Techniques and Considerations in Combining Their Use

In order to meet the requirements of the 1977 Clean Air Act regarding attainment of the National Ambient Air Quality Standards for particulate matter, EPA has been preparing guidance for use in identifying and quantifying source contributions to measured ambient particulate matter concentrations. Many analysis techniques and models have been developed for the purpose of source apportionment. Receptor models are those that are based primarily on data gathered at the receptor where the ambient concentrations are measured. Source or dispersion models are those that are based primarily on data gathered at the source.

Guidance for using source apportionment techniques has been compiled by EPA into the Receptor Model Technical Series. The first four volumes in the Technical Series have primarily addressed receptor model source apportionment techniques. Volume I (EPA-450/4-81-016a), entitled "Overview of Receptor Model Application to Particulate Source Apportionment," introduces the concept of receptor models and briefly discusses the various types of receptor models and their applications. Volume II (EPA-450/4-81-016b), pertains to the "Chemical Mass Balance" model and provides information on model theory, data requirements and case studies of the application of the model to emission control strategy development. Volume III (EPA-450/4-83-014), the "User's Manual for (a) Chemical Mass Balance Model," documents a computer program that performs source apportionment using the weighted least squares and other optional forms of the mass balance equations. The user's guide provides a complete program listing, an example set of input and output data and further discussions of model theory and use.

Volume IV of the series (EPA-450/4-83-018), "Summary of Particle Identification Techniques" gives an overview of the methods and equipment generally used in particle characterization for source apportionment studies. The discussion includes sampling and analytical methods, choice of filter media, particle properties and source fingerprints, costing and method selection criteria.

The present volume, (EPA-450/4-84-020), "Source Apportionment Techniques and Considerations in Combining Their Use," provides guidance for the coordinated use of the various receptor and source model techniques in source apportionment activities. Summary discussions of the available receptor and source models are presented. The use of the models is discussed in a phased approach starting with analyses of low complexity and cost and proceeding to analyses of greater complexity and cost, but which produce more quantitative results. Input data requirements for each phase and example case histories are provided.

This report was prepared by TRC Environmental Consultants, Inc. for the Office of Air Quality Planning and Standards in fulfillment of Contract Number 68-02-3514, Work Assignments 21 and 34. The contents of this report are reproduced herein as received from the contractor. The opinions, findings, and conclusions expressed are those of the authors and not necessarily those of the U.S. Environmental Protection Agency. The mention of product names does not constitute endorsement by the U.S. Environmental Protection Agency.

ABSTRACT

Receptor Model Technical Series

Volume V

Source Apportionment Techniques and Considerations in Combining Their Use

The Clean Air Act of 1977 requires the development of State plans for the attainment of the National Ambient Air Quality Standards (NAAQS) for particulate matter. In order to assist in this effort, EPA has been preparing guidance for use in identifying and quantifying source contributions to measured ambient particulate matter concentrations. Much of this guidance has been incorporated into the Receptor Model Technical Series. This document is the fifth in the series. Many air sampling techniques, analytical procedures and models have been developed for the purpose of apportioning source contributions. The models that have been developed for this purpose are of two general types: receptor models that are based primarily on ambient measurements and related analytical techniques, and source or dispersion models that are based primarily on source emissions data and atmospheric dispersion calculations.

The purposes of this document are to 1) summarize the information which will facilitate the design of a source apportionment study using a combination of receptor and source models, 2) identify approaches in which receptor models can be used to increase the reliability of source (dispersion) models, and 3) identify ways and conditions under which the aforementioned receptor models can be used in concert (without a dispersion model) to provide reliable estimates of source category contributions to ambient particulate matter

problems. To achieve these purposes, this volume 1) discusses models which identify source contributions to receptor concentrations, their input data, the assumptions on which they are based, and the effects of typical deviations from those assumptions, 2) identifies measurements which these models require, their availability, the additional assumptions imposed by these measurements, and the effect of their precision and accuracy on modeling results, and 3) presents approaches, pertaining to three levels of analysis detail, for the optimum combinations of models and measurements in practical situations and illustrates these protocols with case studies.

EXECUTIVE SUMMARY

This document is intended as a source of information on the use of various combinations of source apportionment methods to determine the relative contribution of pollution sources to measured levels of particulate matter in the ambient atmosphere. The apportionment of source contribution is especially important in nonattainment situations so that cost-effective strategies can be developed for source control to achieve attainment. This document is intended for air quality specialists in all levels of government and in industrial and consulting establishments to provide guidance in selecting and implementing combinations of source apportionment methods.

Receptor-oriented models based on unique properties of source emissions and source-oriented models based on dispersion equations are both imperfect representations of complex physical realities. By combining receptor- and source-oriented models the skilled analyst can learn more about the nature of the nonattainment situation and can possibly develop quantitative source-receptor relationships which will greatly increase confidence in the choice of control strategies.

Modeling involves a five step process. The five steps are 1) development, 2) verification, 3) evaluation, 4) application, and 5) validation. This volume is concerned primarily with the model application step of this process, but it does not provide step-by-step procedures for the application of composite methods because of the wide range of techniques available and the attendant uncertainty in the reliability of the results. Rather, it describes the most important available source- and receptor-oriented models and how they

may be used in combination to develop a source apportionment strategy. The reader is directed to published literature for the detail on each of the models described and its method of application.

Both non-computer and computer source (dispersion) models are described. The computer models identified and summarized include: PTMAX, PTDIS, PTPLU, PTMTP, CRSTER, MPTER, RAM, CDM, ISC, and Valley. The use of these models in applications ranging from screening to detailed analyses is described. The ISC model has the greatest application to a composite source apportionment approach because of its ability to handle particle deposition.

The receptor models described include some that provide qualitative and some that provide quantitative source apportionment results. The most important of the quantitative receptor models are those based on mass or element balance. Also discussed are other types of quantitative and semi-quantitative receptor models including factor analysis, multiple linear regression, optical microscopy, scanning election microsopy and x-ray diffraction.

Mass balance techniques require both ambient and source composition data to produce a quantitative source apportionment solution. Factor analysis models require a qualitative knowledge of the composition of source emissions in order to identify which factors are associated with each source type. Multiple linear regression analyses require a separate determination of tracer elements or constituents attributable to specific sources. The source compositions gained by factor analysis and multiple linear regression can be used as input to the mass balance model to quantify source contributions.

Optical microscopy can provide semi-quantitative source apportionment if particles associated with specific source types are large enough to have characteristics that can be identified by visual inspection (e.g. specific minerals). Included among the properties used to identify particles are color, shape, index of refraction and bi-refringence. Automated scanning electron microscopy coupled with energy dispersive x-ray analysis provides data on particle shape, elemental content and particle sizing to smaller physical diameters than can be observed by optical microscopy. X-ray diffraction can be used to identify and distinguish among chemically-identical, coarse, crystalline particles.

The qualitative receptor modeling techniques discussed include:

- Background Concentration Analyses
- Historical Trends and Monthly Variation Analyses
- Weekday/Weekend and Wet Day/Dry Day Analyses
- Analyses of Frequency Distributions and Tests for Lognormality
- Episode Day Analyses and Spatial Mapping
- Correlation Coefficients and Time Series Analyses
- Wind Trajectories and Pollution Roses

Five factors must be considered in the design of a source apportionment study. These are 1) the time frame of the problem, 2) the existing data base, 3) the nature of the problem, 4) the applicability of complementary methods, and 5) resource availability. This volume discusses the interrelationships among these factors and provides an assessment of various complementary uses of receptor and dispersion models.

Source apportionment studies are organized here into a three level format, with Level I being the simplest and least costly and Level III being the most complex and expensive. This approach was recommended by the participants at the second Mathematical and Empirical Receptor Models Workshop (Quail Roost II) held in March 1982 in Rougemont, North Carolina. The levels are considered to be a continuum in which the first step is based on existing measurements. Then, depending upon the resources and data available, and the objectives of the study, additional measurements are made and more complex models are applied until a satisfactory level of confidence in the study conclusions is achieved. A summary of the three level approach is also provided.

Several case studies are described that represent all three levels of complexity and combinations thereof.

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1.0 INTRODUCTION

The identification of the sources of ambient suspended particulate matter and the quantification of their contributions are necessary to devise strategies to attain National Ambient Air Quality Standards (NAAQS). Currently, the standards of concern pertain to total suspended particulate matter (TSP), but EPA is considering the proposal of a revised NAAQS based upon particles of less than 10 µm aerodynamic diameter (PM_{10}). The transport of particulate matter from source to receptor is a complicated phenomenon and various models and measurement systems have been formulated to represent it. While these models and systems enhance the understanding of reality, no model can be a perfect representation of that reality. No mathematical formulation can include all of the variables which are known to affect particle concentrations at a specific point and time. No measurement system is capable of providing values to all variables which can be included in the models. However, one must work within the limitations of the models and measurements to develop the best possible approach to source apportionment.

Since source apportionment analyses require both measurements and models, it is somewhat difficult to develop a cost-effective procedure to quantify the source contributions to pollutant concentrations at a receptor. A model, by itself, cannot always be judged good or bad, or right or wrong, in a general way. The model and the measurement processes, (which supply the data on which the model operates and the values with which its results are compared), and the physical situation being evaluated must all be considered when designing a source apportionment study, to ensure that an adequate level of confidence in the study results will be provided. The purposes of this document are to 1) summarize the information which will facilitate the design of a source apportionment study using a combination of receptor and source models, 2) identify approaches in which receptor models can be used to increase the reliability of source (dispersion) models, and 3) identify ways and conditions under which the aforementioned receptor models can be used in concert (without a dispersion model) to provide reliable estimates of source category contributions to ambient particulate matter problems. This document, of necessity, contains abbreviated discussions of many subjects, so references are provided if greater detail is needed.

To achieve these purposes, the objectives of Volume V in the Receptor Model Technical Series are:

- Discuss models which identify source contributions to receptor concentrations, their input data, the assumptions on which they are based, and the effects of typical deviations from those assumptions.
- Identify measurements which these models require, their availability, the additional assumptions imposed by these measurements, and the effect of their precision and accuracy on modeling results.
- Present approaches, for three levels of analysis detail, for the optimum combinations of models and measurements in practical situations and illustrate these protocols with case studies.

This volume is limited to a discussion of analyses involving particulate matter, although some of the techniques presented herein may be applicable to analyses of other pollutants. This document does not attempt to define a specific policy for combining the use of receptor and dispersion models or for reconciling differences among results; however, approaches for comparing receptor and dispersion model results are presented.

Volume V is intended to supplement the previous four volumes in the Receptor Model Technical Series (U.S. EPA 1981a, 1981b, 1983a, 1983b) and the Guideline on Air Quality Models (U.S. EPA, 1978a). Since it has become common practice to do so, in this volume the term "model" is applied to all the analytical (and measurement) techniques used in source apportionment analyses. Techniques that allocate source contributions based primarily on source emissions data and dispersion calculations are called source or dispersion models. Techniques that primarily use ambient measurements and related analytical methods to apportion source contributions are all called receptor models.

Much of the information on the following pages has been drawn from existing studies and reports, many of them sponsored by U.S. EPA. The selection of the information included from these studies has been made by the authors and the reader is referred to the complete reference for greater detail. It is hoped that the selection is of sufficient detail to allow the user of Volume V to conceptually design a source apportionment study with limited support from other documents. However, it will often be necessary to refer to the more detailed documents to carry out many of the specific analytical procedures described herein.

Similarly, the protocols described here are illustrative rather than definitive. It is impossible to anticipate all of the objectives, available resources, and site-specific requirements of an individual aerosol source-apportionment study. Because of the uncertainties inherent in all of the models, it is recommended that more than one be used in forming the basis for potentially costly decisions. As Cooper (1981) points out:

> "The information provided by these models is circumstantial in nature and the results from a single interpretive approach at this stage of model evaluation may be insufficient to develop the level of confidence required to support strong action or clear decisions. The objective of source apportionment studies must be to build a strong enough bridge of circumstantial information to quantitatively relate a source to an impact."

For this reason, the protocols proposed here combine various models and measurements in levels ranging from basic analyses using existing data to a custom-designed measurement and analysis study. Each level of application requires greater resources, but should yield results of higher confidence. These combinations of source apportionment techniques, from which this volume draws its title, are more likely ". . . to provide decision makers with confidence that their actions will result in improved air quality." (Cooper, 1981).

Two types of models are considered in this composite approach: source and receptor models. Both are derived from the same basic physical principles, but they differ in the measurements on which they operate. Source models (for general reference see U.S. EPA, 1978a; Turner, 1970, 1979; Hanna, et al., 1982) infer an effect from a cause. They combine pollutant emission rates and meteorological variables to calculate the pollutant concentration at a set of receptors. Receptor models (for general reference see U.S. EPA 1981a; Macias and Hopke, 1981; Dattner and Hopke, 1983; Henry, et al., 1983) infer a cause from an effect. They combine aerosol properties measured at receptors with those typical of potential sources to calculate the contributions which each source could have made to the receptor concentrations. Both types of models are applicable to the composite source apportionment approach, but the greatest potential benefit results from the combined use of source and receptor models.

Three types of measurements are required as input to these models: emission rates and meteorological variables are required by source models, and emission compositions, meteorological variables and ambient concentrations are required by receptor models. The availability, quality, and quantity of these measurements will dictate which of the source and receptor models is most applicable to a situation and the accuracy, precision, and validity which can be expected from the model results.

This introduction has served to state the objectives of Volume V in the Receptor Model Technical Series, place it into perspective with other volumes in the series and EPA guidelines, and to preview its contents. Section 2 identifies the five step modeling process and the source and receptor models which can be used for aerosol source apportionment studies. The measurements they require are specified, and the major assumptions imposed by the models and their measurements are listed. In several cases, verification and evaluation studies have been conducted with these models, and relevant results are drawn from them. These studies indicate the accuracy of model results which can be expected under ideal and typical conditions.

Section 3 deals with the measurements required by the models specified in Section 2. Since measurements constitute the major cost of a model application, already available or easily attainable measurements are identified whenever possible. All measurements required by both source and receptor models possess an accuracy and precision which should be translated, where possible, to the model result. Typical accuracies and precisions of the required measurements are stated in Section 3.

In Section 4, the considerations in method selection are discussed and possible combinations of source and receptor models and measurements are proposed at three levels of detail. Each level is more costly, but more accurate and precise, than the previous level. The first level uses existing measurements. The second level generally requires additional analyses of existing samples and may require some new monitoring. The third level requires possible development and deployment of new measurement systems.

Although three levels of analysis detail are discussed, this document is not a workbook or procedures manual because problems differ in their time frame, nature, existing data base contents, model applicability and resource availability.

Applications of the protocols in each level are discussed in a series of case-studies in Section 5. The important points made in Volume V of the Receptor Model Technical Series are summarized in Section 6.

2.0 SOURCE AND RECEPTOR MODELS

2.1 The Five Step Modeling Process

Numerous air quality simulation models of both the source and receptor variety have been proposed over the last ten years. However, many of these are variations of the same conceptual formulation and the most useful of these concepts have been incorporated into a relatively small number of standardized computer programs which are available to the user community without requiring major modification.

The use of any model involves a five step process: 1) development, 2) verification, 3) evaluation, 4) application, and 5) validation.

Model development is complete when the equations constituting the model have been derived from basic physical principles, all simplifying assumptions have been stated, and a standardized procedure, including operations manual and computer programs, have been written and agreed upon. This volume does not address model development beyond that which has already taken place.

Model verification (after Fox, 1981) consists of comparing the values of the model calculations with corresponding measured values for the same variables under conditions for which deviations from model and measurement assumptions are known to be the minimum possible. One can expect no better agreement between calculated and measured values than that obtained by the model verification.

Model evaluation (also after Fox, 1981) involves the comparison between corresponding calculated and measured quantities under conditions of known deviations from model and measurement assumptions. The evaluation results in a correspondence between changes in the model calculations (with respect to that achieved by the model verification) and a quantifiable deviation from each assumption. The reader is referred to the results of the Quail Roost II

Workshop for further discussion of model verification and evaluation (Stevens and Pace, 1984).

The results of these verification and evaluation studies are important and should be part of the knowledge of every model user. Model verification studies have compared calculated and measured concentrations under the most favorable modeling conditions; in most cases they show significant discrepancies even under these best-case conditions. These discrepancies are typical of the minimum differences between model calculations and reality which a modeler can expect to find in less controlled but practical situations. Evaluation studies have compared model-calculated and measured concentrations under less-favorable but known conditions. When these conditions are similar to those under which the modeler is working, the discrepancies found in the evaluation studies may be representative of those which will be found in the modeler's application.

Model development, verification and evaluation are not the responsibility of the routine model user. They are typically performed on a generic basis by the developer of the model or by EPA with the results made available to the user. Significant progress has been made in the verification and evaluation of many models.

The application step involves acquisition of the necessary measurements, running the model, and interpreting the results with respect to the objectives of the study. This application step is the focus of this document.

The validation step consists of determining the extent to which model and measurement assumptions were met for the particular application, and ascertaining from the model evaluation studies the quantitative effects of deviation from those assumptions on the model results. Criteria for model validation are discussed further in Stevens and Pace, (1984). The application and validation steps of the process are the responsibility of the user.

In the following subsections, the presently available source and receptor models for relating source contributions to receptor concentrations will be associated with their basic assumptions and the measurements they require. Summaries of their verifications and evaluations are provided.

2.2 Source Models

Source models predict pollutant concentrations in the atmosphere using emissions and meteorological data. Most source models presently in use are Gaussian kinematic models. These models are based on assumptions of a steady-state atmosphere and a Gaussian or normal distribution of pollutants in the horizontal and vertical directions. Source models employ equations that calculate the dispersion of emissions in the atmosphere and are therefore also called dispersion models. Source models are now widely used in regulatory applications, especially to determine the effects of proposed new sources or changes in the emission characteristics of existing sources. Since this document is part of the receptor model technical series, the discussion of source models is limited to their use in developing control strategies for State Implementation Plans (SIPs). Also, although many verification and evaluation studies have been performed for source models, these studies are not given as detailed treatment in this document as are such studies for the receptor models.

2.2.1 Non-Computer Source Modeling Approaches

Simple source models can be used to obtain estimates of the maximum potential contribution of individual sources. Commonly used methods for obtaining such estimates can be found in the Workbook of Atmospheric

Dispersion Estimates by Turner (1970) and in Volume 10R of the Guidelines for Air Quality Maintenance Planning and Analysis (U.S. EPA, 1977a). As shown in these references, reasonable estimates of aggregate source contributions can also often be determined using simple "box" models where total source emissions are calculated to be dispersed within defined geographic boundaries based on mean climatological conditions. Such models are most appropriate for non-reactive pollutants and areas with standard meteorological regimes. They are most often used with gross emission estimates for multiple sources in an area but could be used in single source applications. They are generally not appropriate for pollutants such as particulate matter, especially for larger time-distance scales, since factors such as washout and settling enter as important considerations.

2.2.2 Computer Based Models

Most new sources are presently reviewed for their air quality impacts using computerized dispersion models. Dispersion models are also often used to determine air quality impacts from aggregate emissions on a regional basis for air quality planning purposes. Guidance regarding the use of dispersion models in contained in EPA's Guideline on Air Quality Models (U.S. EPA, 1978a). EPA has developed a series of models which are recommended for use in air quality permitting and planning applications. Models developed by the State of Texas are also currently recommended for such use. The EPA and Texas models are available on computer tape as part of Version 5 of EPA's User's Network for Applied Modeling of Air Pollution (UNAMAP) Series (U.S. EPA, 1983c). Table 2-1 provides a summary of the features, input, output and applicability of many of these widely-used computerized source models and further discussions of these models follow.

TABLE 2-1

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
1. PTMAX	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • Calculates point of maximum concentration for various wind speed/stability combinations • Point sources only	• Point source emission rate, release height, effluent velocity and temperature	• Table of maximum hourly concentrations and distances to maximum concentrations	• Screening for locating areas of highest concentrations
2. PTDIS	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • Calculates concentrations at user defined source to receptor distances • Point sources only	• Hourly wind speed, temperature, stability and mixing height (non-preprocessed) • Source to receptor distances • Point source emission rate, release height, effluent velocity and temperature	• Maximum hourly concentrations at discrete receptor distances	• Screening for calculating concentrations at specific receptor distances
3. PTPLU	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • Calculates point of maximum concentration for various wind speed/stability combinations • Adjusts wind speed for plume height • Point sources only	• Point source emission rate, release height, effluent velocity and temperature	• Table of maximum hourly concentrations and distances to maximum concentrations	• Screening for locating areas of highest concentrations
4. PTMTP	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • User defined source and receptor locations	• Hourly wind speed and direction, temperature, stability and mixing height (non-preprocessed) • Source and receptor locations	• Hourly concentrations at each receptor • Averages of the hourly concentrations at each receptor	• Estimate concentrations from worst-case hourly meteorology • Point sources only • Short term averaging periods only

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
4. PTMTP (cont'd)	• Point sources only	• Point source emission rates, release heights, effluent velocities and temperatures		
5. PAL	• Pasquill-Gifford dispersion in the horizontal and vertical • Point, area, and line sources • User defined source and receptor locations • Flat terrain only • Can simulate curved line sources • Urban mode stability class adjustments	• Hourly wind speed and direction, temperature, stability and mixing height (non-preprocessed) • Source and receptor locations • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates, lengths, widths and heights • Line source emission rates, widths and initial horizontal and vertical dispersion values	• Hourly concentrations at each receptor • Averages of the hourly concentrations at each receptor	• Estimate concentrations from worst-case hourly meteorology • Multi-source complexes oo developments in urban areas • Short term averaging periods only
6. CRSTER	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • Collocated sources in center of polar grid • Full terrain subtraction for elevated receptors • Point sources only	• Hourly wind speed and direction, temperature, stability and mixing height (from preprocessor program only) • Concentric ring receptor distances and elevations • Point source emission rates, release heights, effluent velocities and temperatures	• Maximum hourly, 3-hr and 24-hr concentrations • Annual average concentration	• Point sources only • Rural non-complex terrain • Short or long term averaging periods
7. TEM-8	• Pasquill-Gifford dispersion in the horizontal and vertical • Dispersion coefficient adjustments for various averaging times	• Hourly wind speed and direction, temperature, stability and mixing height (non-preprocessed) • Source locations • Receptor grid dimensions	• 50 highest 24-hr average concentrations	• Multi-source flat terrain situations • Short term averaging periods only

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
7. TEM-8 (cont'd)	• Flat terrain only • User defined source locations • Variable size receptor grid • Point and area sources	• Point source emission rates, release heights, effluent velocities, and temperatures • Area source emission rates and grid size		
8. MPTER	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • User defined source and receptor locations and elevations • Variable (user defined) terrain subtraction for elevated receptors • Point sources only	• Hourly wind speed and direction, temperature, stability and mixing height (user defined or from preprocessor program) • Source and receptor locations and elevations • Point source emission rates, release heights, effluent velocities and temperatures	• Same as CRSTER	• Point sources only • Rural non-complex terrain • Short or long term averaging periods
9. COMPLEX I	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5°) dispersion in the horizontal • Briggs plume rise • Plume terrain impaction options • User defined source and receptor locations and elevations • Point sources only	• Hourly wind speed and direction, temperature, stability and mixing height (user defined or from preprocessor program) • Source and receptor locations and elevations • Point source emission rates, release heights, effluent velocities and temperatures	• Similar to MPTER	• Point sources in complex terrain • Short or long term averaging periods

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
10. COMPLEX II	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • Plume terrain impaction options • User defined source and receptor locations and elevations • Point sources only	• Hourly wind speed and direction, temperature, stability and mixing height (user defined or from preprocessor program) • Source and receptor locations and elevations • Point source emission rates, release heights, effluent velocities and temperatures	• Similar to MPTER	• Point sources in complex terrain • Short or long term averaging periods
11. RAM	• Choice of Pasquill-Gifford or McElroy-Pooler (urban) dispersion in the horizontal and vertical • Briggs plume rise • User defined source and receptor locations • Point and area sources • Flat terrain only	• Hourly wind speed and direction, temperature, stability and mixing height (user defined or from preprocessor program) • Source and receptor locations • Point source emission rates, effluent velocities and temperatures • Area source emission rates, side lengths and heights	• Same as CRSTER	• Point and area sources in urban areas • Non-complex terrain • Short or long term averaging periods
12. ISCST	• Pasquill-Gifford dispersion in the horizontal and vertical • Briggs plume rise • User defined source and receptor locations and elevations • Point, area and volume sources • Full terrain subtraction for elevated terrain • Urban mode stability class adjustments	• Hourly wind speed and direction, temperature, stability and mixing height (user defined or from preprocessor program) • Source and receptor locations and elevations • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates, side lengths and heights	• Similar to CRSTER • Sources may be aggregated in user defined groups	• Point, area, volume (line) sources in rural or urban areas • Most appropriate for large, multi-source industrial complexes • Non-complex terrain • Short or long term averaging periods

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
12. ISCST (cont')	• Building wake effects algorithm • Particle deposition calculations • Emission rate variability	• Volume source emission rates, side lengths, heights, and initial horizontal and vertical dispersion values • Building dimensions for point source downwash effects • Particle size distribution information • Emission variation parameters		
13. Valley	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5^o) dispersion in the horizontal • Briggs plume rise • Fixed receptor field with adjustable source locations • Point and area sources • Sums concentration over stability/wind rose joint frequency • Fixed meteorology for short term calculations • Variable receptor terrain height	• Stability/wind rose (STAR) deck • Source locations • Concentric ring receptor distances and elevations • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates, side lengths and heights	• Average concentrations on receptor field	• Single or multiple sources in complex terrain • Short or long term averaging periods
14. AQDM	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5^o) dispersion in the horizontal • Sums concentration over stability/wind rose joint frequency	• Stability/wind rose (STAR) deck • Source and receptor locations • Point source emission rates, release heights, effluent velocities and temperatures	• Average concentrations at each receptor	• Urban multi-source flat terrain situations • Long term averaging periods

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
14. AQDM (cont'd)	• Point and area sources • User defined source and receptor locations • Flat terrain only	• Area source emission rates, side lengths and heights		
15. TCM-2	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5^0) dispersion in the horizontal • Sums concentration over stability/wind rose joint frequency • Point and area sources • User defined source locations • Variable size receptor grid • Flat terrain only	• Stability/wind rose (STAR) deck • Source locations • Receptor grid dimensions • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates and grid size	• Average concentrations at each receptor	• Multi-source flat terrain situations • Long term averaging periods
16. CDMQC	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5^0) dispersion in the horizontal • Briggs plume rise • User defined source and receptor locations • Point and area sources • Sums concentrations over stability/wind rose joint frequency • Flat terrain only • Allows adjustment factor to each concentration	• Stability/wind rose (STAR) deck • Source and receptor locations • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates, side lengths and heights	• Average concentrations at each receptor • Adjusted concentrations	• Urban multi-source flat terrain situations • Long term averaging periods

TABLE 2-1 (Cont'd)

SOURCE MODELS

Model	Features	Input Data	Output Data	Common Applicability
17. ISCLT	• Pasquill-Gifford dispersion in the vertical • Sector average (22.5°) dispersion in the horizontal • Briggs plume rise • Sums concentration over stability/wind rose joint frequency • User defined source and receptor locations and elevations • Point, area and volume sources • Full terrain subtraction for elevated terrain • Urban mode stability class adjustments • Building wake effects algorithm • Particle deposition calculations • Emission rate variability	• Stability/wind rose (STAR) deck • Source and receptor elevations and locations • Point source emission rates, release heights, effluent velocities and temperatures • Area source emission rates, side lengths and heights • Volume source emission rates, side lengths, heights, and initial horizontal and vertical dispersion values • Building dimensions for point source downwash effects • Particle size distribution information • Emission variation parameters	• Average concentrations at each receptor • Sources may be aggregated in user defined groups	• Point, area, volume (line) sources in rural or urban areas • Most appropriate for large multi-source industrial complexes • Non-complex terrain • Long term averaging periods

2.2.2.1 PTMAX, PTDIS, PTMTP

PTMAX, PTDIS and PTMTP (U.S. EPA, 1983c) are three models used for screening purposes in relatively simple situations. PTMAX and PTDIS are used in single source analyses. PTMTP can be used to analyze multiple sources. Generally PTMAX is used to obtain an estimate of maximum impacts for a single point (i.e., stack) source. PTMTP is used to obtain maximum combined impacts from several point sources under worst-case meteorological conditions.

2.2.2.2 PTPLU

PTPLU (U.S. EPA, 1982c) has been developed by EPA as an improved version of the PTMAX model and has generally replaced PTMAX in screening analyses. PTPLU determines maximum concentrations from a single point source under various wind speed/stability combinations. PTPLU can accommodate non-zero receptor elevations and includes the effects of wind speed increase with height, gradual plume rise, and buoyancy-induced dispersion. PTPLU is often used to select receptor points for sophisticated hour-by-hour model calculations.

2.2.2.3 PAL

The PAL model (U.S. EPA, 1978b) is the only EPA developed model which will accept point, area, and line sources. Area sources are used to represent groups of small sources and line sources are used to represent roads and other similar sources. This gives the model considerable flexibility in analyzing complex urban sources and proposed developments. User-defined hourly meteorological data for worst-case situations are generally used as input. Only flat terrain is simulated.

2.2.2.4 CRSTER

The CRSTER model (U.S. EPA 1977b) calculates impacts from single or collocated point sources using hourly meteorological data generally developed from National Weather Service (NWS) observations. Usually a full year of meteorological data is used for a single analysis. The CRSTER user's manual (U.S. EPA, 1977a) summarizes results of several studies which evaluated the model's accuracy. Most of these studies showed reasonable agreement between measured and modeled values but noted problems in determining background and obtaining reliable concentrations in elevated terrain situations.

2.2.2.5 TEM-8

TEM-8 (Texas Air Control Board, 1979) is a model developed by the Texas Air Control Board for calculating short-term ambient concentrations of pollutants from point and area sources. TEM-8 does not use a one year hour-by-hour meteorological data set as is common to EPA-developed short-term models. Instead TEM-8 allows up to 24 user-generated meteorological scenarios. The input meteorological data are assumed to be representative of a given time period ranging from 10 to 180 minutes.

The concentration prediction algorithms in TEM-8 involve the use of the standard Gaussian distribution of concentrations in the horizontal, but, the horizontal distribution values used in the model are believed to be appropriate for ten minute averaging times only. Meteorological scenarios which produce concentration predictions for other than ten minute averaging periods use horizontal concentration distribution values which are adjusted from the ten minute values, depending upon the averaging time.

TEM-8 calculates concentrations from normalized concentration/emission (X/Q) values using a table look-up procedure that is dependent upon plume height, stability, downwind distance, and averaging time. This procedure saves considerable computation time in comparison to calculating concentrations using the Gaussian equation as is done in most EPA-developed models.

TEM-8 predicts pollutant concentrations on a rectilinear grid with spacing determined by the user. All receptors are assumed to have an elevation equal to the stack base. Pollutant deposition or transformation can be simulated using an exponential decay function.

2.2.2.6 MPTER

MPTER (U.S. EPA, 1980a) is a dispersion model similar to CRSTER which allows analysis of multiple distinct point sources located in level or gently rolling terrain. It also uses a year of hourly meteorological data and affords greater flexibility in data input and output.

2.2.2.7 COMPLEX I and II

Complex I and II (U.S. EPA, 1983c) are two models used for dispersion modeling analyses of point sources located in complex terrain. They use a year of hourly on-site or NWS preprocessed meteorology in the CRSTER format. Complex I and II differ in their computation of horizontal dispersion. Complex I assumes pollutants are dispersed uniformly into a 22.5 degree downwind sector, while Complex II uses a standard Gaussian horizontal distribution. Inputs and outputs for Complex I and II are similar to MPTER.

2.2.2.8 RAM

The RAM model (U.S. EPA, 1978c) is used to analyze multiple point and area sources on an hour-by-hour basis. A one year meteorological data set similar to the CRSTER input is employed by RAM. RAM is currently the only EPA model to include urban dispersion coefficients, developed by McElroy and Pooler. RAM is recommended for use in urban areas to determine the aggregate impacts of multiple point and area sources.

2.2.2.9 ISC

The Industrial Source Complex (or ISC) model (U.S. EPA, 1979a) is used to calculate air quality impacts from single or multiple point, area, or volume source emissions. Volume sources are used to provide an improved representation of certain elevated area sources such as roof monitors and storage piles. Both a short-term (ISCST) and a long-term (ISCLT) version of the model are available. The ISCST model uses hourly meteorological data derived from NWS observations in a CRSTER preprocessed format. Meteorological input to ISCLT consists of a joint frequency-stability wind rose developed from one or more years of hourly NWS observations. The ISC models have a number of options involving input and output data and contain a great deal of flexibility regarding input source information. Two capabilities unique to ISC among EPA developed models are the ability to account for building wake effects and particle deposition caused by gravitational settling. The ISC model's superior capabilities for handling various types of sources and particle deposition make it the most useful model for source/receptor modeling applications. An evaluation of the ISC model performed by EPA showed that predicted and observed calculations for both the deposition and building wake options generally produced agreement within a factor of two, although it was noted that appropriate specification of the building dimensions affecting initial plume dispersion was difficult (U.S. EPA, 1981c).

2.2.2.10 Valley

The Valley model (U.S. EPA, 1977c) is used to determine pollutant concentrations at receptor locations with receptor elevations greater than the height of the emission point being modeled. Multiple non-collocated sources as well as area sources can be modeled with Valley. The Valley model computes annual average concentrations based on a stability wind rose similar to ISCLT. Twenty-four hour concentrations that are assumed to represent high second-high values for a year are calculated using worst-case meteorology. An analysis of the Valley model given in the Valley user's guide describes a general overprediction when the model is used in its short-term mode compared to measured SO_2 concentrations.

2.2.2.11 AQDM

The AQDM model (TRW, 1969) calculates annual average concentrations of sulfur dioxide or particulate matter in urban areas. Both point and area sources may be used as input. Concentrations can be determined at a program-generated rectangular grid of receptors and at discrete receptors, both of which can be user-defined. Meteorological input consists of a stability-wind rose similar to that used by other long term models. However, in AQDM the two stable categories, E and F, and combined into a single stable condition. AQDM uses the standard Gaussian dispersion curves but it is assumed that urban heat island effects produce neutral stability when the input meteorological data indicate stable conditions. Thus only the vertical dispersion values for stabilities A through D are used in the model. Horizontal dispersion is assumed equal throughout a 22.5 degree downwind sector for all stabilities. AQDM uses the Holland plume rise formulation, rather than the Briggs equations used in other EPA models. AQDM has a calibration feature, similar to that in CDM, that allows for adjustment of predicted concentrations based on actual measured values from a monitoring network.

2.2.2.12 TCM-2

TCM-2 (Texas Air Control Board, 1980), is a model developed by the Texas Air Control Board for use in their permitting analyses. TCM-2 calculates long-term (seasonal or annual) concentrations of pollutants on a user-defined rectilinear grid. A stability wind-rose is generally used as meteorological input. The model can handle both point and area sources and allows for exponential pollutant decay. A least-squares algorithm is provided for calibrating predicted concentrations to observed values. TCM-2 is a flat terrain model, i.e., all receptors are assumed to be located at the elevation of the stack base.

The TCM-2 algorithm employs several techniques which reduce the computation time of the model compared to other long-term models such as CDM. These include use of a table look-up scheme for determining χ/Q dilution values, use of a single mean wind speed for a given stability and wind direction, and the omission of mixing height-induced multiple reflection calculations. The user's guide presents a discussion of these computation-reducing features.

2.2.2.13 CDM/CDMQC

The CDM/CDMQC model (U.S. EPA, 1973, 1977d) is used to calculate multiple point and area source impacts in urban areas on a quarterly or annual average basis. A stability wind rose is used as meteorological input to CDM. CDM does not include terrain effects in its algorithms. A useful feature of this model is the ability to adjust predicted concentrations based on a linear regression against monitoring data from a network of stations. The CDM user's guide describes an example study in which this adjustment was used to offset over-predictions of SO_2 concentrations.

2.3 Receptor Models

Receptor models can be used for a variety of purposes. This document is limited to discussion of applications that allocate ambient concentrations of particulate matter to the contributing sources. In the context of the development of SIPs, receptor models are used for the purpose of formulating and demonstrating the effectiveness of control strategies to attain and maintain NAAQS. Since there is great complexity involved in the transport and transformation of emissions from multiple sources to the particulate matter measured at a receptor site, no single model has superior applicability to all source apportionment analyses. In addition, more than one model should be applied in any given analysis to ensure the reliability of the analysis results and the cost-effectiveness of any control strategies subsequently developed.

The various quantitative and semi-quantitative receptor models that have been developed and applied to accomplish this purpose are listed in Table 2-2 along with their positive and negative features, required input data, their outputs, and the commonly available measurements to which they are applied. As noted earlier, the detail presented here is considerably greater than that given for source models in keeping with the title of this technical series. Reference is made to other publications documenting the specific procedures for using a model.

TABLE 2-2

RECEPTOR MODELS

Model	Features	Input Data	Output Data	Common Applicability
1. Chemical Mass Balance	• Quantitative estimates of source contributions • Applies to single or time-averaged samples • Computerized model available from EPA or private contractors with a number of solution methods • Can use non-computerized "tracer" mode for simple solutions when sources have unique properties	• Ambient concentrations of particle properties from one or more samples • Number of source types • Potential contributing source types • Source compositions of source types	• Source contributions	• Fine and coarse samples with x-ray fluorescence (XRF), ion, and other analyses
2. Factor Analysis	• Has potential to identify presence of source contributions • If source emission rates vary independently, if source compositions are constant and dissimilar, and if correlations of concentrations depend only on emissions and not on meteorology, then source compositions can be estimated. • Source contributions can be calculated via mass balance using information gained by factor analysis • Computerized model available on many statistical software systems such as SPSS, SAS, BMDP. • Requires multiple samples	• Ambient concentrations of particle properties from >50 samples • Qualitative knowledge of source compositions	• Number of distinguishable source types • Source compositions • Source contributions (when factor analysis is combined with mass balance)	• Fine and coarse samples with x-ray fluorescence (XRF), ion, and other analyses

TABLE 2-2 (continued)

RECEPTOR MODELS

Model	Features	Input Data	Output Data	Common Applicability
3. Multiple Linear Regression	• One unique "tracer" property is chosen for each source considered; it should have negligible concentrations in other source emissions. • If source compositions are constant and correlations of concentrations depend only on emissions and not on meteorology, then fraction of tracer property in source composition can be estimated. • Source contributions can be calculated via mass balance. • Solution algorithm is part of most computer libraries • Requires multiple samples	• Number of source types • Unique tracer property for each source type • Ambient concentrations from >50 samples	• Quantity of tracer property in source composition • Source contributions	• Fine and coarse samples with x-ray fluorescence (XRF), ion, and other analyses • Hi-vol samples with atomic absorption (AA), microscopic and/or organic analyses
4. Optical Microscopy	• Provides estimates of source contributions • Provides size classification • Applies to single samples, but multiple samples more beneficial • Requires trained analyst	• Physical/optical properties of source particles • Ambient samples (particles >1-2 μm only)	• Source contributions • Size classifications	• Hi-vol samples

TABLE 2-2 (continued)

RECEPTOR MODELS

Model	Features	Input Data	Output Data	Common Applicability
5. Scanning Electron Microscopy	• Provides estimates of source contributions • Provides size classification • Applies to single samples, but multiple samples more beneficial • Requires trained analyst • Can be computerized	• Elemental/physical properties of source particles • Ambient samples	• Source contributions • Size classifications	• Hi-vol samples
6. X-Ray Diffraction	• Provides estimates of source contributions of crystalline materials • Applies to single samples • No sample preparation	• X-ray diffraction properties of crystalline source particles • Ambient samples	• Source contributions	• Hi-vol samples

2.3.1 Chemical Mass Balance Model

The mass balance model (Friedlander, 1973; Watson, et al., 1981; Cooper and Watson, 1980; Henry, et al., 1983) solves a set of equations to determine the combination of source contributions that provides a best fit to measured ambient concentrations of selected particulate matter components (i.e., chemical elements, ions, or compounds; size fractions; or other measured properties.) The mass balance model, which is also known as the chemical mass balance (CMB), chemical element balance (CEB) and chemical species balance model in the literature, requires information concerning the composition of both source emissions and ambient concentrations. Refined results can be obtained if the component concentrations are compiled on a particle-size specific basis.

In the mass balance equations, the total ambient concentration (C) of a component (i) from all sources (j) is set equal to the linear sum of the products of 1) the component's fractional mass contribution (F) to the source's total emissions, and 2) the source's fractional mass contribution (S) to the total ambient concentration measured at the receptor:

$$C_i = \Sigma F_{ij} S_j$$

Thus, if the total ambient particulate matter concentration (within the specified size range) and the (corresponding) ambient and source component concentrations are measured, source contributions to the receptor can be calculated.

The simultaneous solution of the mass balance equations is an integral part of the mass balance model. There are a number of available solutions to the mass balance equations. The tracer solution (Miller, et al., 1972, Kneip, et al., 1972) assumes certain tracer properties are unique to each source type. It is the simplest solution and unlike other solution methods requires no computer. The intent of the linear programming solution (Mayrsohn and Crabtree, 1976; Henry, 1977, Hougland, 1983) is to find optimum values for the source contributions. The ordinary weighted least squares solution (Friedlander, 1973), which weights variables by the inverse squares of the precisions of the ambient concentrations, has been supplemented by the more general effective variance least squares solution (Britt and Luecke, 1973; Dunker, 1979; Watson, 1979; Watson, et al., 1983). The effective variance solution includes weighting by the precisions of the source compositions as well as weighting by the precisions of the ambient concentrations. The intent is to weight the most precisely known measurements most heavily in arriving at a least squares solution yielding source contributions to observed ambient concentrations of particulate matter. The effective variance least squares solution is more valid than the ordinary least squares solution only if the precision of the source data are known. Such data are often missing or of poor quality. A ridge regression solution (U.S. EPA, 1983a) is intended to minimize instabilities in a least square solution when two or more source categories being considered have similar chemical compositions. In ridge regression, the goal is to introduce a small bias into the solution in order to achieve a large reduction in the random error, so that the total error is reduced. As Henry has shown (1982), the introduction of such a bias can result in an underlying source matrix that is not representative of the true source profiles. Ridge regression should not be used indiscriminately, as if its application would automatically eliminate all problems caused by multicollinearity, since it cannot be guaranteed that its use will produce a better solution than conventional least squares in every application.

The assumptions of the mass balance model are (Watson, 1982):

- Compositions of source emissions are constant over the period of ambient and source sampling.
- Components (e.g. chemical species) do not react with each other, i.e., they add linearly.
- All sources with a potential for significantly contributing to the receptor have been identified and have had their emissions characterized.
- The number of sources or source categories is less than or equal to the number of components.
- The source compositions are linearly independent of each other.
- Measurement errors are random, uncorrelated, and normally distributed.

Model verification and evaluation studies have been conducted and published by Watson (1979), Gordon, et al., (1981); Currie, et al., (1983); and Dzubay, et al., (1983). These studies consist of 1) comparison of different mass balance solutions operating on the same measured data, 2) comparison of different solutions applied to simulated data with the known source contributions from which the data are derived, and 3) analytical examination of the solutions of the mass balance equations. The results of those evaluations as they relate to the above assumptions are discussed in Appendix A.

The selection of source types, source compositions and aerosol measurements is an integral part of the mass balance model application. This selection is often dictated by the measurements which are or can be made available. These measurements are the subject of Section 3.

Volume III of this technical series (U.S. EPA, 1983a) describes a chemical mass balance model algorithm developed for EPA. Other, similar mass balance model algorithms have also been developed. These models are usually applied by allowing the user to add various source types and types of ambient data into one of the solution methods until most of the measured properties at a receptor are accounted for by the source contributions. Unfortunately, in some cases, several mathematical "solutions" can be found which "account" for these receptor properties equally well, with no detrimental effects on the least squares fitting criteria. In intercomparisons of a number of mass balances solutions applied to a 9-day average, size-segregated particle data base from Houston, Texas, Dzubay, et al., (1983) found several different solutions which were considered acceptable by the participants. In similar intercomparisons using simulated data, a number of different, acceptable solutions were found to the mass balance equations also (Currie, et al., 1983), as was the case when multivariate techniques were used. Watson (1979) observed that "The receptor model tells what could be the contributors, not necessarily what the contributors are." The results from the Houston data base analysis reaffirm that it is advisable to have a qualitative knowledge of the contributing sources before seeking to obtain quantitative source contribution estimates using the mass balance model.

The major contributors to average concentrations in the simulated data set were estimated, for the most part, to be within ±30 percent of their true values. Minor contributors were often within a factor of two (Currie, et al., 1983). Although the true contributions in Houston were unknown, the range of values for most source types was less than a factor of two (Dzubay, et al., 1983). A further note of caution on the Houston analyses, as well as for analyses conducted previously in other cities (U.S. EPA, 1981b), is that sulfate, nitrate, carbon and crustal material are defined by chemical characteristics and not their sources. Therefore, continued research is required to obtain parameters that will account for the generation, transformation and removal of particles during transport from source to receptor.

The uncertainty of the mass balance results is probably comparable on average to that expected of source models intended to accomplish the same purpose. Some aspects of this problem are discussed for the simulated data set (Currie, et al., 1983) by Gerlach, et al., (1982), and more generally by Henry (1982).

2.3.2 Factor Analysis

Factor analysis solutions can be obtained by different methods. Classical factor analysis or principal component analysis can be applied to ambient sample composition measurements at a receptor to produce a set of uncorrelated factors which are associated with various sources. Under certain circumstances, these factors can be interpreted as being representative of specific sources and, using additional steps, can provide estimates of source emission compositions. Factor analysis for receptor modeling requires elemental and chemical or other constituent concentration measurements at receptors, but does not require quantitative characterization of source emissions. However, some qualitative information on sources and the characteristics of the local meteorology are necessary to interpret the factors (Cooper and Watson, 1980). The derived source emission compositions can then be used in a mass balance to determine the relative contribution of different sources to each observed concentration.

Factors are derived from the correlations of observed particulate matter or other ambient concentration measurements that represent different time periods of sampling at a receptor location. Factor analysis assumes that the composition of particulate matter from a given source remains constant over all of the ambient samples and that inter-species correlations are due to changes in source strength. Advantages of factor analysis include the ability to distinguish among sources which contain the same constituents (in different proportions), the ability to identify previously unsuspected sources and no requirement of quantitative source composition measurements. Disadvantages include added complexity, the need to impose arbitrary constraints on source emission composition in order to obtain a unique solution, and the need for detailed ambient composition data for a relatively large set of ambient measurements. However, the latter can provide information on sources over the course of a season (Kneip, et al., 1983; Morandi, et al., 1983) or year (Kleinman, et al., 1980; Thurston, 1983) if sufficient samples are taken to satisfy statistical constraints. For mass balance analyses, a limited (one or more) number of samples are required in each season, but more source testing may be necessary.

The factor analysis model (Henry, 1977; Kleinman, et al., 1980; Hopke, 1981; 1983; Henry, et al., 1983) consists of 1) forming a correlation matrix by summing over aerosol samples (known as "Q mode") or over aerosol properties (known as "R mode"), 2) finding the eigenvalues and eigenvectors of the correlation matrix, 3) discarding a number of eigenvectors and eigenvalues which are deemed insignificant; the number of values remaining are examined and interpreted for identification of source types, 4) forming linear combinations of eigenvectors which represent source compositions or choosing representative tracers, and 5) using these source compositions in the mass balance equations. Each of these steps includes a variety of options, the selection of which differentiates one factor analysis model from another.

Correlation or covariance matrices around the mean or the origin can be used (Rozett and Peterson, 1975; Duewer, et al., 1976) in R-mode, or in Q-mode (Alpert and Hopke, 1980; 1981). These matrices can contain as many aerosol properties and as many samples as desired (available), though Henry, et al., (1983) estimate that the minimum number of samples needed is:

$$m > 30 + \frac{n + 3}{2}$$

where m = number of samples
n = number of aerosol properties

enry, et al., (1983) conclude that if 20 aerosol properties are used, an dequate correlation matrix can be formed only if at least 42 samples are vailable.

The determination of eigenvalues and eigenvectors is performed by a ariety of computer subroutines which are common to most computer libraries, nd though individual algorithms vary, they yield essentially the same results.

The selection of the number of eigenvalues to retain is open to question. lpert (1980) proposed five criteria: 1) eigenvalue equal to 1, 2) chi square,) Exner function, 4) root mean square (RMS) error, and 5) indicator unction. Alpert (1980) found most of these tests indicated the same number f significant aerosol sources in practical applications, but that for certain ases they were inconsistent. Hopke (1982) warns that "Many statistical ackages, including BMDP and SPSS, set the eigenvalue of 1 criterion as efault and do not examine additional factors unless the default is pecifically counter-manded. This procedure can lead to exclusion of ignificant factors." Thus an appropriate test for selecting the number of ontributing sources from the available eigenvectors needs to be developed. or principal component analysis, Roscoe, et al., (1982) have suggested that or eigenvalues of less than 1 to be included, the variance of a rotated actor should be greater than 1.

Selected eigenvectors can be more easily related to source compositions fter a vector rotation has been done by a 1) varimax, 2) quadrimax, or 3) arget transformation method. The target transformation method has been shown to be useful for aerosol receptor models by Hopke, et al., (1983). However it is constrained by the selection of the profile used as a target. Henry (1977) chose targets which were actual source compositions similar to those known to be present in the study area by minimizing the sums of the squares between target and rotated vector coordinates. The new vector coordinates were taken to be a more refined estimate of the true source composition.

Recently Thurston (1983) used principal component analysis for source identification in Boston, Massachusetts. In this instance, the factor scores were adjusted to absolute zero and the resultant adjusted factor scores were used to conduct a mass balance analysis.

2.3.3 Multiple Linear Regression

Regression techniques provide a straightforward method for characterizing the composition of a set of concentration measurements. Multiple linear regression provides a least-squares solution which apportions a total or size-segregated particulate matter concentration among a set of chemical elements and/or other constituents. The general form of the solution is:

$$Y = A_0 + A_1 X_1 + A_2 X_2 + . . . A_n X_n,$$

where Y is the observed concentration, the X_i's represent the various constituents, and the coefficients A_i are calculated to provide a least squares fit to the data.

Unlike the mass balance method, multiple linear regression, taken alone, does not require data regarding the composition of the emissions from sources, and does not directly identify source contributions to ambient concentrations, unless proper selection techniques (e.g., factor analyses) are used to select the constituents that are analyzed. The analyst must separately determine which sources are responsible for emitting a specific element or chemical species and ensure that tracers are available for use in the analyses.

The assumptions of the multiple linear regression model taken alone include the following:

- All of the important constituents of ambient particulate matter have been identified and measured.
- The contributions of different constituents are linearly independent of one another.
- For any given set of constituent values (X_i's), the observed concentration values (Y's) are normally distributed.

The multiple linear regression results will rank the independent variables (constituents) in order of importance, for explaining variations in the total concentration, and will also identify those constituents which play no significant role in explaining variations in the total concentration.

The above is a very rudimentary approach to the analysis of source apportionment data. However, if multiple regression techniques are coupled with procedures that independently identify the X_i's, the regression analyses can be applied to mass balance calculations. Kleinman, et al., (1980) published work for New York City that used cluster and factor analysis to identify source profiles and subsequently selected fairly unique tracers for use in a stepwise regression model to apportion the ambient particulate matter mass. Subsequently, Kneip, et al., (1983) and Morandi, et al., (1983) used the Factor Analysis/stepwise Multiple Regression Receptor Model (FA/MRRM) to apportion size-selected samples for New York City and the Airborne Toxic Elements and Organic Substances (ATEOS) site in Newark, New Jersey, respectively. Hopke, et al., (1983) applied scaling factors to his source profiles obtained from target transformation and used a regression model to attribute the ambient mass measurements. As mentioned in the previous section, Thurston (1983) has developed adjusted (absolute) principal components for source types that were subsequently used in a regression model to apportion the ambient mass.

2.3.4 Optical Microscopy

Examination of particles collected on a filter medium using an optical microscope provides insights into the origins of particulate matter (Draftz, et al., 1980; Crutcher, 1982; U.S. EPA, 1981a; 1983b). In the hands of an experienced microscopist, optical microscopy (OM), also known as light microscopy (LM) and polarized light microscopy (PLM), can often yield a semi-quantitative determination of the relative contributions of source types if the categories of sources are few in number and produce completely different types of particles, e.g., distinguishing between particles of mineral origin such as road dust and particles produced by combustion processes (Throgmorton and Axtell, 1978).

Particles may be examined *in situ* on the filter medium with or without immersion oil or may be removed with adhesives, probes, or ultrasonically for examination under more controlled conditions. However, any method in which the particles are removed from the original filter media may compromise the representativeness of the analysis and produce biased results.

Particle sizes below about 1 or 2 µm cannot be readily identified by optical microscopy since these particle sizes begin to approach the wave-length of visible light. Since ambient particle size distributions are typically bi-modal, consisting of two families of particles, with the mode of one greater than about 10 µm and the mode of the other less than about 2 µm, most fine particles cannot be identified using optical microscopy.

Particles can be examined by both reflected and transmitted light. Transmitted light may be polarized by any of a number of orientations allowing the skilled microscopist to identify a variety of mineral species. Although color photographs of known particle types are helpful to the microscopist in making particle and, hence, contributing source identifications, (McCrone, 1973), many analysts prefer to have source emission samples collected within the study area.

The various material characteristics that are examined include structure, transparency, color, and optical properties. The identification system is used with a series of tables such as those found in Kerr (1959) which associate the observed properties or parameters with a list of materials having those properties. Some of the properties observed are: color, habit (shape and form), cleavage, index of refraction, isotropic versus anisotropic, birefringence, and uniaxial versus biaxial.

Particles that have been identified are grouped within categories such as combustion products, minerals, biological material (e.g., pollen), rubber, and eventually a miscellaneous or unknown category.

In order to assign a quantitative value to the relative abundance of a given species it is necessary to carry out a particle size distribution for each of the identified categories. Then, if a particle density can be assigned to each category, the relative percentage by weight for each category can be estimated.

Several attempts have been made to evaluate the reproducibility of microscopic analysis or particle collections by such techniques as inter-laboratory analysis of blind replicate samples. The results show wide disagreement in results among analysts. Factors contributing to differences in the results of analyses by skilled microscopists include: 1) lack of common agreement concerning particle removal or in situ examination; 2) disagreement over source classification groupings, 3) different particle sizing and counting methods, and 4) statistical counting errors (e.g. if 10^3

particles of 5µm diameter and 2.5 g/cm^3 density are examined, only 0.3 µg out of a typical deposit of 10^5 µg, or less than 10^{-3} percent of the sample, will be examined).

Further details on the use of optical microscopy in source apportionment studies can be found in Volume IV of this series (U.S. EPA, 1983b).

2.3.5 Scanning Electron Microscopy

Another method used to provide particle-specific information is the scanning electron microscope (SEM). An automated scanning electron microscope (ASEM), which produces digitized particle images, can be used to overcome many of the problems associated with individual particle analyses. A scanning electron microscope combined with automated image analysis and X-ray spectroscopy (SAX), also known as computer controlled scanning electron microscopy (CCSEM), can be used to provide simultaneous measurement of individual particle size, shape and elemental composition.

CCSEM combines three analytical tools under computer control: 1) the scanning electron microscope, 2) an energy dispersive spectrometry (EDS) x-ray analyzer and 3) a digital scan generator for image processing (Casuccio, et al., 1983).

In the CCSEM, a finely focused electron beam impinges upon the sample surface. The interaction of the electron beam with the sample produces secondary and/or backscattered electrons that are used to create a viewing image, while the x-ray emission is monitored to determine the elemental chemistry of the particles.

The automated image analysis of CCSEM is normally conducted in the backscattered mode. The backscattered signal is sensitive to differences in atomic number and is thus suited to the analysis of particles. Solid-state backscattered electron detectors are positioned above the sample; their individual signals are amplified and then summed to produce the final backscattered electron signal.

The computer compares the image intensity at each point with a threshold level. This comparison is used to determine whether the electron beam is "on" a particle (above threshold) or "off" a particle (below threshold). If the signal is below the threshold level, the computer selects a new (x,y) coordinate and directs the beam in a preset pattern of rotated diagonals to determine the dimensions and shape of the detected feature. The pattern is repeated twice, once to locate the feature centroid and once to determine the lengths of the diagonals. For each feature, the maximum, minimum, and average diagonals are stored, along with the centroid location. The centroid is used to prevent double counting.

To classify and distinguish different particle types, it is essential to determine the elements contained in each particle, along with the relative intensities for each particle. Once the electron beam is positioned on a particle, the x-ray spectrum is collected. All elements heavier than sodium are simultaneously detected. The computer's classification routine identifies the most significant peak(s) and assigns each particle to the group of particle types having the same major elemental constituent(s). The relative intensities of the major and minor elements in the spectrum are then used to assign each particle to a specific particle type within the group. Particle types (e.g., spherical iron and cenospheres) may also be classified by the aspect ratio or shape factor. The absence of elemental peaks or a low peak-to-background signal causes the particle to be classified as carbon. Particles found on ambient filters are compared to those on source emission filters (preferably collected within the study area) to identify contributing sources and determine source contributions.

One advantage of this technique is the ability to rapidly analyze large numbers of particles, thus overcoming the statistical limitations inherent in optical microscopic methods. Because each particle analysis requires two to five seconds, 1000-2500 particles may be examined in a two-hour period. (Although this is a larger number of particles than is usually analyzed optically, it is on the order of 0.001 percent of the deposit on a filter sample and may not be statistically representative of the entire sample.) This method can analyze particles from any filter medium if particles are removed prior to insertion into the microscope. Care must be taken to ensure that the removed particles are representative of the original sample (Kelly, et al., 1980). Nuclepore or Teflon filter media are usually required for the *in situ* examination of particles. However, *in situ* analysis requires lightly loaded filters, which may not be practical in some instances.

Further discussion of this technique can be found in Volumes I and IV of this series (U.S. EPA, 1981a; 1983b) and in Johnson, et al., (1983).

2.3.6 X-Ray Diffraction

The x-ray diffraction (XRD) technique is also a method used to provide particle information. The method depends upon the wave character of x-rays and the regular spacing of planes in a crystal. X-rays impinging on the crystal are diffracted in a manner that is unique to that crystalline structure. The diffraction "fingerprint" obtained can be compared to a library of data (e.g., American Society of Testing Materials, 1955) and the structure identified. Various automated cameras and devices are now in use to accelerate this process.

This technique is specifically utilized to identify the crystalline phases present in a sample: e.g., quartz, calcite, dolomite, halite, lead ammonium sulfate. It can provide a direct identification of such sources as pavement minerals, soil minerals, ores, pigment, cement, metal oxides, asbestos, abrasives, sulfates and nitrates, and indirect identification of road and sea salt. Sometimes it is the only method available for determining which of the possible polymorphic forms of a substance are present: for example, carbon in graphite or in diamond. Differentiation among various oxides such as FeO Fe_2O_3, and Fe_3O_4, or between materials present in such mixtures as KBr + NaCl, KCl + NaBr, or all four, is easily accomplished with x-ray diffraction, whereas chemical analysis would show only the ions present and not the actual state of combination. XRD can also identify the presence of various hydrates.

XRD is basically a qualitative analysis method, although it is also adaptable to quantitative applications since the intensities of the diffraction peaks of a given compound in a mixture are proportional to the fraction of the material in the mixture. However, direct comparison of the intensity of a diffraction peak in the pattern obtained from a mixture is difficult. Corrections are frequently necessary for the differences in absorption coefficients between the compound being determined and the matrix.

The method is applicable to most filter media and no sample preparation is necessary. A loading of at least 200 $\mu g/m^3$ on the filter is optimum, but not necessary.

Further information on this technique may be found in Willard, et al., (1974); Kuwana, (1980); U.S. EPA, (1981a, 1983b); and Johnson, et al., (1983).

2.3.7 Preliminary or Qualitative Receptor Models

The foregoing subsections describe some sophisticated techniques that can provide quantitative estimates of source attribution. Application of those techniques requires that the user have either specialized equipment and training or a significant understanding of mathematical and statistical manipulation of data. The methods described in this subsection require spatial and/or temporal correlation of aerometric data plus a moderate understanding of statistics and may be used to supplement the results of other receptor modeling or may be used to draw inferences from available data on categories of sources contributing to measured particulate matter levels. These methods use historical data for particulate matter, collected using both standard high volume (hi-vol) and size selective air samplers, together with local meteorological data to establish background levels, trends, interrelationships between station values, geographical and wind direction-stratified patterns, and relative influence of non-traditional sources. It can be assumed that many of these analyses will have been completed prior to conducting more complex receptor modeling simply because they represent a means of developing common understanding of the receptor data and their interrelationships.

These qualitative receptor modeling techniques include the following:

- Background Concentration Determinations
- Historical Trends
- Frequency Distributions
- Tests for Lognormality
- Monthly Variations
- Weekday/Weekend Analysis
- Wet Day/Dry Day Analysis
- Episode Day Analysis
- Spatial Mapping
- Correlation Coefficients
- Time Series Analysis
- Wind Trajectories and Pollution Roses

Each of these are described in the following paragraphs. Further details on these methods and their interrelationships as source apportionment methods can be found in Brookman and Yocom (1980), Throgmorton and Axetell (1978), and U.S. EPA (1983d).

2.3.7.1 Background Component Determinations

For purposes of developing a control strategy for particulate matter, background concentrations must be taken into consideration.. The method that federal regulations (Section 51.13c) specify for estimating background is to use a concentration measured at a non-urban site that is in or near the study area and is unaffected by nearby emission sources. This concentration is assumed to be composed of material that is transported into the study area from external sources over which the area (i.e., the local control agency) has no control, plus material generated within the study area from natural and agricultural sources. Unfortunately, an ideal, unaffected, non-urban site in the area of study does not always exist. As an alternative, the background particulate matter level can be established by developing a composite particulate matter rose where data gathered at several monitoring sites are averaged based on the frequency of winds coming from selected directional sectors, as described below.

To remove the influence of the study area sources on particulate matter levels within the study area, only data collected at selected monitoring sites located at the far edges of the study area, during periods when the sites are upwind of the study area sources, are chosen for analysis. The particulate matter concentrations at these sites are then screened for all sampling days with a wind persistence factor (Heidorn, 1978) above a selected value (e.g.,

≥0.71*). These daily concentrations are then classified by wind direction sector and the sector average of each data set is calculated for each site. A composite particulate matter rose is constructed utilizing the wind direction sector-average concentration values from the selected sites. To determine a weighted average background level, the percent of time the wind blows from each directional sector is used. The average particulate matter level for each directional sector is multiplied by the frequency of wind from that sector and the results are summed in order to give the weighted average.

The weighted values obtained are usually composed of particulate matter from natural and agricultural sources, transported secondary particulate matter and locally-generated particulate matter from such sources as residential heating, vehicle exhaust, reentrained road dust, tire rubber, and vegetative burning. In most instances, the influence of the latter sources will be relatively minor. This background particulate matter composition can be further defined by analysis of the material collected on samples selected to represent background conditions.

Particle size-fractionation analyses can be used to help differentiate between transported particles (usually in the fine fractions) and locally-generated particles (usually in the coarse fractions). Chemical composition analyses can be used to differentiate between particle types and thus help define their origins. In this manner, a background particulate matter level for the study area can be established. In subsequent analyses, this background level can be applied uniformly to data at all sampling sites within the study area.

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*Wind persistence factor is defined as the ratio of the vector averaged wind to the average wind speed over the 24 hour sampling period. A factor near 1.0 indicates a wind that blows consistently from one direction during the entire sampling period. A persistence factor ≥0.71 is equivalent to an hourly wind direction deviation of 45°.

2.3.7.2 Historical Trends

Using the historical particulate matter data, the yearly arithmetic and geometric means are calculated for each monitoring site. These means are then plotted as a continuous function of year for each station in order to identify the occurence of sudden changes at that particular station. It is usually helpful to subtract the study area background level from the annual mean at each station before plotting or else to plot the background level for each year alongside the monitoring site means. This will serve to either factor out or allow for an evaluation of the effect of year-to-year variations in meteorological conditions (e.g., precipitation) on the sampling days. This analysis technique can provide the following types of information.

- A large change in the yearly particulate matter levels at only one site can indicate a local source, such as a construction project, starting up or shutting down. It could also be indicative of a siting change.
- A large change in the yearly particulate matter levels at several sites in a large geographical region can indicate a major particulate matter source starting up or shutting down or undergoing a major change in operations.
- Gradual changes in the yearly particulate matter levels at a particular site or several sites can indicate the effectiveness of implemented control measures or the gradual deterioration of a control program.

2.3.7.3 Frequency Distributions

Analysis of the frequency distribution of the ambient data will often provide insight into the mix of contributing sources. A common methodology involves grouping the data into concentration bins which are then displayed graphically as histograms. If the distribution is bi-modal or shows extreme values (outliers) of much larger concentration than the mass of data, then a directionally dependent effect on that monitor, or intermittent, infrequent source or other similar causes for the anomolous values may be suspected.

2.3.7.4 Tests for Lognormality

The presence of predominant local sources can often be confirmed by testing the ambient concentration data for lognormality. This can be done by applying statistical tests (e.g., Kolmogorov-Smirnov) to the data or by plotting the data (Larsen, 1971). In the latter case, the percentage of measurements greater than a selected particulate matter concentration is plotted as a function of the logarithm of that particulate matter concentration. If the resulting curve is nearly a straight line, the observations are lognormally distributed and the site is likely subject to large-scale or general influences (i.e., many sources). If there is a major local influence, such as a nearby stack or a strong area source in a specific direction with respect to the sampling site, then the data will most likely either not exhibit lognormality or will deviate from it at the plot extremes (Larsen, 1971).

2.3.7.5 Monthly Variations

Several years of particulate matter concentration data are averaged by month and plotted to show the monthly and seasonal variations that exist at each of the sites. Corresponding plots of background concentrations can be used to show the effects of changing meteorological conditions. An abnormally high winter average can be an indication of heavy traffic influence due to the combination of longer morning inversion periods, cars idling while cold, road sanding/salting operations and increased space heating, especially by wood stoves. A high summer level can be an indication of dry surface soil in conjunction with agricultural activity or the increased use of school playgrounds. High summer and fall concentrations may also be caused by secondary aerosols, construction activities, pollen, leaf burning, etc. This can be verified by chemical analysis.

A variation of this analysis can be performed where the monthly average plots are grouped for stations that are similar in character or in close proximity. This helps to determine whether these groups of stations are influenced by regional-scale, urban-scale or neighborhood-scale sources. Two stations in an urban area might exhibit similar seasonal particulate matter patterns, indicating that an urban- or regional-scale source is the major contributor. On the other hand, one station might have a higher overall particulate matter concentration, indicating a local- or neighborhood-scale source influence.

2.3.7.6 Weekday/Weekend Analysis

During weekends, driving is typically done in the middle of the day when dispersion conditions are at their best. During weekdays, peak driving is typically done in the early morning (0630-0900 hours) and late afternoon (1500-1800 hours) when dispersion conditions may be poor, thus keeping traffic-suspended particulate matter in the vicinity of the point of generation in a relatively undiluted condition. Weekday and weekend traffic volumes also differ considerably. By computing the arithmetic averages for weekday and weekend periods as well as Saturday and Sunday individually for each site, a measure of the influence of traffic on ambient particulate matter levels can be obtained. Most industries operate on a 7 day week, but if a source does operate on a 5 day week or has a lengthy shutdown, then its contribution may also be estimated from this type of time series averaging analysis. Other sources with a weekend/weekday dependence could confound this analysis. The analysis may be enhanced if weekdays/weekends with similar meteorological conditions are compared, but additional work is required to stratify the particulate matter data by meteorology.

2.3.7.7 Wet Day/Dry Day Analysis

It may be assumed that on days with sufficient snow cover, with greater than 0.5 centimeters of precipitation, or following days with greater than 0.5 centimeters of precipitation, the principal contributions to particulate matter levels are traditional sources, home heating, vehicle exhaust, and material transported from outside the study area. The rain and snow suppress the majority of the local fugitive and reentrained dust. These days are defined as "wet" days and all other days as "dry" days. The meteorological data for the study period are examined and the particulate matter levels at each site on wet days are then averaged and compared to the average particulate matter levels on the dry days. The differences give a first approximation of the reentrained dust and local fugitive emissions contributions at each of the sampling stations. In an extension of this analysis, the particulate matter levels on days with snow cover can be averaged versus days without snow cover. Such an analysis is often helpful in approximating the effect of total control of windblown dust from sources such as inactive storage piles. When conducting these analyses, care must be taken to consider the effects of winter sanding and salting in those areas where this is practiced. Results may be misleading in such instances.

2.3.7.8 Episode Day Analysis

Days are selected on which higher than typical particulate matter concentrations are recorded throughout an area. The meteorological data are examined to determine the possible influence of inversions, stagnation conditions, days since last significant precipitation event, etc. Large-scale sources, most likely outside the study area (i.e., long-range transport), are possible reasons for such regional-scale emission events. Examples might be dust storms, forest fires, volcanos, etc.

2.3.7.9 Spatial Mapping

In this method, the particulate matter data obtained on all sampling days, or only those days when the wind persistence factor (the ratio of the vector averaged wind to the average wind speed) is above a selected value (e.g., ≥ 0.71), are sorted by wind direction category (compass sector). The particulate matter concentrations for each sector are averaged for each site based on the number of observations and the averages are then used to form maps representing particulate matter concentrations associated with winds from each of the compass directions. If sampling is conducted at a number of sites in the study area, these maps may help identify the location of contributing sources, based on the sites and wind directions associated with the highest average concentrations. Such maps may be particularly useful for PM_{10} studies since the spatial variability of PM_{10} is less than that of TSP. However, in most urban situations the maps may be misleading because predominant, very localized influences can overwhelm the contributions from sources with more widespread impacts.

2.3.7.10 Correlation Coefficients

A correlation coefficient between two variables indicates a co-variation of the individual measurements of those variables. Many times a common cause of this co-variation, owing to meteorological or emissions variability can be inferred. If concentrations between sites display high correlation coefficients (i.e., they track nearly identically), then the monitoring stations could be influenced by the same types of sources or changes in pollution dispersion. This would be the case where there are regional-scale influences.

Conversely, low correlation coefficients between sites could be caused by local influences. An example would be the case where one monitor is located adjacent to a steel mill while another monitor is near a highway interchange.

2.3.7.11 Time Series Analysis

The time series analysis is another valuable technique for obtaining insight into source/receptor relationships. In one such analysis, the 24-hour concentration measurements for all the sites in the study area can be plotted versus time on the same graph. The concentrations will usually vary in a similar manner. Sites and periods which do not vary similarly are indicative of events that occur on a neighborhood scale. Time series plots can also be prepared to compare changes in particulate matter concentrations to changes in meteorology (e.g. wind direction, wind speed) and other parameters.

2.3.7.12 Wind Trajectories and Pollution Roses

Pollution roses, which depict the average particulate matter concentration for various wind directions, are constructed for each site for each of the study years. They can be based on concentration averages for eight or sixteen compass points for all sampling days or only those sampling days possessing a pre-selected wind persistence factor.

These roses are useful in associating average pollutant concentrations with a particular wind direction or directions. They are capable of showing the following types of influence from sources:

- Lack of any specific directional effect of sources or background stations.
- Diffuse influence of distant industrial complexes.

- Combination of diffuse influence from distant sources and nearby sources.
- Influence of nearby large sources.

As an aid in performing the analysis, the percent of time the wind blows from a particular direction (e.g., persistence $\geq$0.71) is determined from the available wind data. This wind frequency can then be combined with the pollution rose information to determine the particulate matter level contribution from a particular compass sector. The value of such analyses depends on the representativeness of the available meteorological data, as discussed in Section 3.3. A good example of the use of pollution roses and wind trajectories is the work performed by Gordon (1980).

3.0 AN EVALUATION OF EXISTING MODEL INPUT DATA

3.1 Overview

, The application of either a source or receptor model requires the acquisition of input data. Generally these input data include source data relating to emission strengths and characteristics, meteorological data, and ambient measurements for the pollutant(s) of concern. Quite often, acquiring input data is the most costly part of any model application. However, there is a large amount of existing data available for use in model applications, and often the objectives of a study can be met without the need for further measurement programs. Frequently, a source or receptor modeling application can be designed around an existing data base. It is useful to examine existing data to determine if further measurements are needed to implement a given application. Review of existing data to determine their quality and validity is necessary before use of the data in any modeling application.

The general types of data used by source and receptor models are shown in Table 3-1. Further discussion of these data are provided in the following subsections.

3.2 Source Data

Source data have generally been compiled in emission inventories, which contain a listing of all recorded sources for a given area. The data contained in emission inventories can vary widely depending upon who has compiled the inventory and the purpose for which it was compiled. Thus it is advisable to review the initial purpose of an inventory before using it in a given application.

TABLE 3-1

GENERAL DATA REQUIREMENTS OF SOURCE AND RECEPTOR MODELS

Types of Data	Source (Dispersion) Models		Receptor Models	
	Screening Analyses	Refined Analyses	Qualitative Analyses	Quantitative Analyses
Emissions				
Emission rates	X	X		
Release heights	X	X		
Source configuration parameters	X	X		
Source locations		X	X	
Size distributions		X		X
Particle compositions		X		X
Meteorology				
Wind directions	X	X	X	
Wind speeds	X	X	X	
Atmospheric stabilities	X	X		
Mixing heights		X		
Temperatures		X	X	
Precipitation			X	
Synoptic scale patterns			X	
Ambient Concentrations				
Measured concentrations				X
Particle compositions				X
Particle sizes				X
Spatial & temporal variations			X	

3.2.1 Emissions Inventories

A basic source of emissions inventory information is generally the State (or local) air pollution agencies. These agencies are usually responsible for gathering information on emission sources within their jurisdiction and compiling the information in an appropriate format. Often these agencies will gather and update source information on a more or less continuous basis but will generate updated inventories at fixed intervals, perhaps annually or biannually. Thus it may be necessary to determine whether the information in a compiled inventory is the most recent available. Often areas with special problems, such as areas with a nonattainment designation, have had special attention made to the completeness and accuracy of their inventories.

State and local air pollution control agency emissions inventories may be limited to point sources in some cases. However, information on non-point source emissions is sometimes available from these agencies. Often during the formulation of SIPs, information has been developed concerning area source or aggregated small source emissions. These are sometimes available on a county, town, or gridded square basis. Information that was used in developing these area source values, such as traffic counts, vehicle miles travelled (VMT), miles of paved and unpaved roads, and population densities are sometimes available. Aggregate fuel consumption statistics are often developed for various types of fuels during SIP development, and these may be broken down to county or grid square values.

There are three reasons for exercising caution when using area source or fugitive emissions inventories: 1) the data used in SIP or nonattainment plan development may have been valid only for the time period when the SIP was generated and may need significant updating, 2) the emission estimates are generally based on emission factors that are imprecise, and 3) the inventories usually do not contain all of the area sources that may be affecting the ambient air quality. The state-of-the-art in emission factors for fugitive dust sources is still far behind that for point sources and estimated emissions can be incorrect. Area source inventories are useful for obtaining an overall picture of the study area, but they may not provide exact modeling results. This is particularly true since most area source inventories only compile the major sources (such as roads, home heating, parking lots) and tend to omit many others (such as industrial fugitive sources, dirt race tracks, drive-in movies) which are potentially important.

The U.S. EPA National Emissions Data System (NEDS) is the standard federal emissions inventory archive. NEDS contains information on both point source and area source emissions. The point source data in NEDS are generally obtained from State and local air pollution agency files. Area source emissions are generally developed on a county-by-county basis from aggregate statistics obtained from State sources. NEDS does not contain the source emissions composition data used by receptor models.

In situations where only a single large source is under study it may be necessary to develop a refined emissions inventory for the given source. Some plants have had comprehensive inventories generated for use in permitting applications or litigation. These are especially useful if reentrained dust and fugitive emission sources were considered or if emissions were based on actual operations rather than rated capacities as is usually done with State inventories. Such in-plant inventories may or may not be available for use in a given study.

There are also several "specialized" inventories which may be of use in a source or receptor modeling study. One type of specialized inventory is the compilation of surface loadings and silt contents of road dust. This is essentially a subset of a general area source or fugitive emissions source inventory and is typically generated for a particular industrial facility. The information on loadings and silt can be used with published emission factors to provide emission estimates for various roadway segments.

Another type of specialized inventory is a compilation of particle size or composition information. This information is obtained using a variety of analytical techniques including optical and scanning electron microscopy, x-ray diffraction, x-ray fluorescence and instrumented neutron activation analysis (INAA). Such information is useful for "fingerprinting" a source so that analyses of the material collected on hi-vol filters can be related to their point of generation.

A third type of specialized inventory is the microinventory which typically presents detailed information on point and area sources in the near proximity of a monitoring station. The distances suggested for including sources in a microinventory are a five mile radius for point sources and a one mile radius for area sources. It is further suggested that all sources within a one mile radius be included, but from one to three miles distance, only those sources greater than or equal to 100 tons per year actual emissions need to be included and from three to five miles distance, only those sources greater than or equal to 250 tons per year need to be included. Microinventories are useful for locating a local source, such as a playground, which may be affecting the recorded levels at a monitoring station but which would not show up in an area-wide inventory. Further information on microinventories can be found in Pace (1978).

3.2.2 Data Quality

The validity of any emissions inventory must be reviewed before its use in any source or receptor modeling application. Validity relates not only to the accuracy of the actual emission values or source parameters but also their representativeness to the application in question. Emission values are often based on annual factors such as fuel consumption, total production, etc. The actual day-to-day operation of a source may vary considerably from these annual average values. In some cases, a short-term inventory may be warranted. In many instances, ambient data are collected for a study period of only weeks or months rather than a full year. The actual operation of important sources during the study period should be reviewed to determine if the inventory data accurately reflect those operations during that time frame. This review should extend to fugitive sources, as well as point sources, to determine if fugitive generating activities, such as unloading or conveying, traffic, and storage pile maintenance occurred with the same frequency as estimated in the inventory.

As discussed earlier, inventories are generally considered valid for a particular point in time and may require updating for a given receptor modeling application. This may involve review of air pollution agency permitting files for inclusion of new sources, reductions due to emission controls, plant shutdowns, and operating limitations. Economic conditions may also affect emissions inventory validity through effects on total plant production, hours of operation, etc. An attempt should be made to include these effects in inventoried data.

3.2.3 Source Emission Compositions

Although few such data are currently available, size-segregated and chemically resolved data are obtained for certain specific sources by analyzing "grab" samples collected from emission control devices, piles of fugitive materials or in-stack sampling. For other sources, these composition data are obtained by analyzing samples collected using sophisticated ground-based plume sampling, dilution stack sampling, vehicle emission sampling or airborne plume sampling. Technical considerations affecting the use of these data include the compatibility between ambient and source sampling periods, the existence of unique (i.e., tracer) emissions, the temporal variability in emission compositions and the similarities in composition of different source emissions. Further discussion of source sampling and emission composition analysis techniques is contained in Gordon, et al., (1983).

One of the biggest impediments to receptor modeling has been the lack of a systemized library of source compositions. EPA is developing such a library (Gordon, et al., 1983; U.S. EPA, 1984). The prerequisites of source compositions for use in mass balance calculations are the following:

- Chemical species and particle size fractions should be the same as those commonly measured at the receptor.
- Sampling conditions should be such that the composition at the source is similar to that received at the receptor. This may require dilution stack sampling or airborne sampling. For certain substances which do not change state or composition with temperature, less expensive grab sampling is adequate.
- Operating conditions of the source must be thoroughly defined since these may affect the emissions compositions. Source configuration, throughput, fuel composition, and temperatures should all be documented.

Very few of the source tests to date meet these criteria. The most commonly used compilations of source compositions are Watson (1979) and Taback, et al., (1979). Appendix B contains a list of sources for which chemical characterizations have been made and some of the references containing the data from those characterizations. As mentioned above, a more detailed library of the chemical characteristics of source emissions is being prepared (U.S. EPA, 1984).

3.3 Meteorological Data

Meteorological data are an important part of any source or receptor modeling study. Meteorology defines the transport conditions under which pollutants move from the source to the receptor, and provides the link between the two. Meteorology can have important effects other than simple transport. Dust suppression due to rain, pollutant buildup due to stagnation, and wind generation of fugitive emissions can have important effects on ambient pollutant concentrations.

3.3.1 Data Quality

A large set of previously compiled meteorological data is available for use in source or receptor modeling applications. However, since meteorological data can be highly variable in space and time, the available data must be evaluated for their representativeness to the given application. The physical scale of the problem under study is especially important. Microscale effects from fugitive sources often require on-site data, whereas multi-state transport studies can use routinely gathered NWS data. If source-receptor relations are being examined, the extent to which measured data reflect conditions at both the source and the sampler should be evaluated, particularly in regard to the sampling height and the mean height of transport. In larger urban areas, multiple meteorological data measurement locations are usually available and spatial averaging may be more appropriate than the values from any single station.

The accuracy and precision of meteorological instrumentation should be evaluated before use of the data in a modeling study. EPA has published specifications for meteorological instrumentation used for on-site prevention of significant deterioration (PSD) monitoring purposes (U.S. EPA, 1980b). Precision is usually a function of the instrument itself and can be obtained from manufacturers' specifications. However, the recording and reduction of measurements may affect the precision of the actual data produced. Meteorological instrument accuracy is generally dependent upon the quality control/assurance (QA/QC) procedures used by the operator. The NWS, which is responsible for gathering most airport meteorological data, as well as the EPA, have developed comprehensive QA/QC procedures for collecting field meteorological data (U.S. EPA, 1982b). Data collected by other agencies should have been subject to similar or otherwise acceptable procedures. Data QA/QC procedures should include an effective procedure for removal or correction of any erroneous values.

3.3.2 Data Sources

The largest source of meteorological data available for source and receptor modeling applications is that data recorded at airports by NWS and Federal Aviation Administration (FAA) observers. These data have been archived at the National Climatic Data Center (NCDC) in both hard copy and computer compatible forms. NWS data are produced by observations made at a once per hour interval. Generally the observer attempts to record a value which is an average over the several minutes previous to the observation time. Thus, since NWS values are not hourly averages and may not represent conditions over the full hour, care should be taken in using these data in combination with hourly average ambient concentrations. Because NWS data are collected, reduced and reported according to standardized QA/QC procedures a generally high level of confidence can be placed in their accuracy. The NCDC archiving facilities also allow generation of large volumes of data in a variety of formats not generally available from other sources.

The U.S. EPA, as well as State and local air pollution control agencies, have often maintained meteorological monitoring networks in combination with their pollutant monitoring networks. Generally the meteorological monitoring is performed at the same location as a pollutant sampler. The collocation of meteorological and pollutant sampling instruments can provide more accurate estimates of near field transport conditions compared to airport data. Pollutant monitoring-based networks generally have several sites in a given region so that overall wind patterns can be deduced. Like the NWS data, monitoring network data are collected and reduced under standardized procedures so a high level of confidence can be placed in their validity.

The EPA and State agencies have from time to time established special monitoring networks during various air pollution investigations. The meteorological data from these studies are sometimes archived at the EPA's National Aerometric Data Bank (NADB). Many of these programs were developed to examine the effects of a single large source and thus give finer spatial scales. Private companies, especially electric utilities, have often supported similar programs, and these data are sometimes archived at State agencies. Data validity from these types of programs should be evaluated by examining calibration procedures and results if they are available.

3.3.3 Meteorological Variables

3.3.3.1 Wind Speed and Direction.

Wind speed and direction are probably the most critical meteorological parameters for source and receptor modeling applications since they define pollutant transport conditions. The most critical factor to be evaluated when using available wind data is their spatial scale of representativeness. Wind speed and direction can change markedly from place to place, especially in the vertical or in areas with varied topography. Airport data are generally taken in large open areas that are often elevated above the surrounding terrain. These data may not represent conditions at industrial sites in river valleys where the topography induces channeling and wind speeds are generally lower. However, airport data may be more representative of the general wind flow over an urban area than is a monitoring site tower located near an individual large source. Many other airports located near coastlines are influenced by seabreezes which do not affect inland industrial sources or urban areas. Generally the spatial scale of representativeness increases with the measurement height. Most airport data are measured at 20 feet above ground and monitoring network data are often measured at 10 meters (33 feet). However, airport data may be more indicative of mean wind conditions due to the open siting requirements of airports. A few monitoring locations have taller towers with instruments at multiple levels. These measurements can sometimes be used to determine wind flow affecting tall stack sources as well as wind direction in the immediate vicinity of the sampler. Rawinsonde balloon measurements can be used for determining long-range transport or regional conditions. Wind measurements made in areas of pronounced topography should be evaluated for the effects of phenomena such as downslope flows, obstacle steering of winds, and increased calms due to flow shielding and stable stratification. These effects may mask the true transport pattern from a source, especially if it is located in a topographic regime separate from the measurement site.

As mentioned earlier, airport observations are actual short-term averages made on a once per hour basis, rather than hourly averages. This is a critical factor for wind speed and direction measurements since the conditions at the time of the observation can easily be anomalous when compared to hourly average conditions. Thus pollutant monitoring network data, which are usually generated as hourly averages, would give a more faithful picture of transport conditions. Airport wind direction observations are recorded to the nearest ten degree value while aerometric monitors can record to single degree values. Wind directions recorded to the nearest single degree may be advantageous when assessing near field transport from closely spaced sources in an industrial complex. Aerometric wind measurements are also generally made with lighter and more sensitive instrumentation than airport measurements.

3.3.3.2 Temperature, Precipitation, and Humidity

Although not as important as wind speed and direction, these variables can affect the generation of fugitive emissions, ambient particulate matter characteristics, and deposition patterns. Temperature, precipitation, and humidity generally do not display the same spatial variability as wind speed and direction, thus evaluation of spatial representativeness is not as critical. Often existing airport data are sufficient for use in a source or receptor modeling analysis. These variables are often not measured at aerometric networks. Temperature and humidity measurements made on towers should be reviewed if ground based fugitive sources are being modeled to determine if the values reflect actual surface conditions. In some cases where a single precipitation measurement is used for a large area, some indication of the rainfall "spottiness" may be necessary to accurately assess dust suppression abilities.

3.3.3.3 Mixing Height

The concept of mixing height is widely used in source models and can be utilized in some receptor modeling analyses as well. Generally, the mixing height is considered to be the height at which the atmospheric lapse rate (the rate of change in temperature with height) suppresses further upward mixing of pollutants. The upward mixing of pollutants may be suppressed when the rate of temperature decrease with height is less than that at lower heights or when the temperature increases with height (producing an inversion). The height/presence of such a lapse rate can only be deduced through vertical atmospheric soundings. The only widely available source of such data is NWS twice per day rawinsonde measurements, which are archived at NCDC, however, some data may be available from utilities, industries, and regulatory or smoke management agencies (e.g., the U.S. Forest Service). In non-mountainous areas use of data from the nearest NWS sounding station is generally adequate because of the broad spatial scale of the data. Capping inversions sometimes occur in valley locations which may not appear in the airport based sounding measurements.

The ideal method of developing mixing heights from balloon data is through individual inspection of each sounding. This may be impractical for a long-term application, however, and the modeler must rely on mixing heights developed from analysis of sounding data by standard algorithms, usually the Holzworth procedure (1972). Some review should be made of the algorithm being used to determine if it is accurately assessing the mixing heights at the location under study.

3.3.3.4 Stability Classes and Dispersion Coefficients

Stability classes and dispersion coefficients are widely used to quantify atmospheric dispersion processes and are central to the formulation of the Gaussian source models discussed in Section 2.2. Stability classes and dispersion coefficients are generated from other meteorological variables. Thus, their degree of representativeness and validity is dependent upon those measurements. A variety of stability classification schemes can be generated from different types of meteorological measurements. The lack of a certain measurement will restrict the user to schemes based on those measurements that are available. The Turner method (1970) develops stability classifications from widely available airport data. Other classification schemes requiring measurement of temperature differences ($\Delta T/\Delta Z$) and the standard deviation of horizontal or vertical wind directions (σ_θ, σ_ϕ) cannot be generated from airport data and can only be used if those measurements are available from aerometric networks or tower sites. A decision on the application of a given stability scheme could be a factor in deciding whether to measure meteorological data on-site.

3.4 Ambient Data

Since this document deals with techniques for apportioning source contributions to receptor measurements, a complete and accurate data base for ambient measurements is probably the most important element for making such an analysis using composite source and receptor modeling techniques. As was pointed out in Section 2.3.7, much can be learned about a nonattainment problem using a structured analysis of existing ambient data.

Particulate matter nonattainment problems are identified using data obtained from networks of samplers, such as hi-vols operated for the purpose of determining compliance with NAAQS. Thus, a basic requirement is to have a data base of several years for a number of fixed stations representing not only the nonattainment area itself but adjoining areas including one or more "background" stations. Data from dichotomous samplers or other types of size-selective samplers, when they are available, can also be especially useful since sampling results can be used directly to infer source category contributions based on size ranges (e.g., large particles tend to be from nearby sources of fugitive dust and small particles tend to be from combustion sources, sulfates or distant sources).

Since trend analysis is an important technique to use on hi-vol data, it is recommended that at least three years of data with a sampling frequency of at least once every 6 days be available for each sampling station to be considered in a trend analysis. It will facilitate the analysis if these data, together with appropriate meteorological data, are archived on a computerized data base and made accessible to manipulation by suitable programs.

Chemical analyses of the particles collected in ambient samples are extremely useful in source apportionment studies. As pointed out elsewhere in this document, chemical and microscopic (optical and scanning electron) examinations of selected samples provide further insight into sources contributing to the measured levels, especially when correlated with meteorological variables.

3.4.1 Data Quality

No ambient sampling methodology is perfect for depicting the actual nature and distribution of particulate matter in the atmosphere. Important factors affecting the validity of particulate matter data include sampling location, instrumentation, sampling schedule, filter material and the methods used to prepare the sample for analysis (U.S. EPA, 1983b; Gordon, et al., 1983).

The siting of samplers is especially important in source apportionment work. Samplers shielded by overhanging trees or nearby buildings can produce non-representative results. Samplers located near busy road intersections, while typical of locations affected by a strong nearby source of fugitive emissions, will be insensitive to the contributions to that location from other types of sources. Guidelines developed by EPA for National Air Monitoring Stations (NAMS) and State and Local Air Monitoring Stations (SLAMS) can be used to evaluate existing sites to determine if they meet acceptable standards for representative ambient sampling (U.S. EPA, 1979b).

Particulate matter sampling is usually performed using hi-vols, sometimes with cascade impactors or size-selective inlets attached, or with dichotomous samplers. Problems with the standard hi-vol include an inability to separate particles by size and imprecise collection efficiencies, as affected by particle size and wind speed and direction. The cascade impactor and size-selective inlet collect material by particle size but retain the other problems of the hi-vol except that sampling with the size-selective inlet is relatively unaffected by wind speed and direction. Dichotomous samplers divide ambient particles into a fine and a coarse fraction but dichotomous sampler collection efficiencies are affected by wind speed and humidity (John, et al., 1983).

Most hi-vol sampling is conducted on an every sixth day sampling schedule and produces samples collected over a 24-hour period. This sampling schedule provides representative samples for a year but obviously omits sampling on 5 out of every 6 days. The 24-hour sampling period precludes the measurement of diurnal or other similar variations in particulate matter concentrations. The amount of particulate matter collected during a 24-hour sampling period may be too much or too little for certain types of constituent analyses. Another consideration is the compatibility between periods of ambient and source sampling.

Most hi-vol particulate matter samples are collected on glass fiber filters. On the whole, such filters are useful for total particulate matter sampling but are less suited for particulate matter constituent analyses. Difficulties with glass fiber filters include particle penetration into the filter and trace element contamination. In addition, the particles on glass fiber filters tend to undergo chemical reactions with each other, with the filter and with gases in the air. These chemical reactions usually involve acid aerosols and acid gases. This problem, called artifact formation, results in erroneous reported concentrations, primarily for the sulfate and nitrate particulate matter fractions. Various types of membrane filters are also used to sample particulate matter. Membrane filters overcome many of the problems associated with glass fiber filters and are the best filters for microscopic analyses, but samples have to be treated carefully because membrane filters are brittle and particles readily fall off them.

Once collected, the particles may be analyzed to determine their composition. In some cases this can be done on the filter, but in others, particles must be removed and inserted into an instrument for examination. Of concern are particles embedded in the filter and particles on top interfering with the analysis of particles underneath.

3.4.2 Data Sources

In the United States most ambient particulate matter data are gathered by federal, State, and local air quality regulatory agencies. Monitoring sites are distributed throughout the nation to monitor compliance with NAAQS. Most of these data are archived using the Storage and Retrieval of Aerometric Data (SAROAD) system in Research Triangle Park, North Carolina (U.S. EPA, 1971). Large amounts of additional data are collected by utilities and industries at and near their facilities. The bulk of these data have been collected using hi-vol samplers, glass fiber filters and an every sixth day sampling schedule. For many years EPA has been compiling particulate matter chemical composition data from designated National Air Surveillance Network (NASN) stations. Such stations are generally a subset of the SAROAD sites operated by State and local agencies. The samples are collected on glass fiber filters using hi-vols operated on an every twelfth day sampling schedule. Chemical composition data are obtained using atomic absorption and wet chemistry methods. EPA has also been compiling particle size and chemical composition data from an Inhalable Particulate Network (IPN) of sampling sites operated in major urban areas (Watson, et al., 1981). Additional comprehensive air quality data are available for St. Louis, Missouri from the Regional Air Pollution Study (RAPS) conducted during the mid-1970s (Strothmann, 1979). Such potential sources of ambient data should be considered before any new sampling is conducted.

4.0 COMPOSITE SOURCE/RECEPTOR MODEL APPLICATION PROTOCOLS

There are many source and receptor models available for use in qualitative and quantitative determinations of the sources responsible for measured ambient particulate matter concentrations. As discussed earlier, the limitations and underlying assumptions of each model are such that all fall short of a perfect representation of reality. Therefore, when seeking solutions to air quality problems, it is highly advisable to use more than one model. A higher degree of confidence can be obtained if several models, operating independently, produce the same results.

4.1 Considerations in Method Selection

This document cannot describe all of the possible combinations of source and/or receptor models that can be used to apportion the contributions of sources to ambient air quality. There are five factors that must be considered before beginning the source apportionment process. These are:

- the time frame of the problem;
- the existing data base;
- the nature of the problem;
- the applicability of complementary methods; and
- the resource availability

Each of these factors is discussed below as a preface to the discussion of a three level approach to source apportionment. Many of the particulars of each factor are discussed in more detail in other sections of this document.

4.1.1 Time Frame of the Problem

The selection of methods must begin by a recognition of the time frame of concern, annual versus 24-hour, which depends on the existing air quality versus the corresponding NAAQS. An annual time frame offers the most flexibility for method selection. Some methods such as the multivariate models (e.g., factor analysis, TTFA and MLR) and the dispersion models work best using multiple samples. If only selected days require consideration in order to develop a control strategy, such methods as chemical mass balance or microscopic analyses may be preferred. However, as described in Section 4.4, an annual time frame study may be performed by merging the analysis results from carefully chosen individual samples.

4.1.2 Data Base

Both ambient and source data bases must be considered. The compatibility of filter material with the needed chemical analyses is important. For instance, the concentrations of certain materials, such as silicon and organic carbon, cannot generally be determined on glass fiber filters because of interferences from the filter material and binder (Pace, 1983). The nature and variability of source emissions may severely limit the use of dispersion models for short-term problems because of the difficulty of reproducing a reliable 24-hour inventory. Generally, receptor models are preferable to dispersion models for short-term retrospective analyses for this reason. This is reflected in Tables 4-1 and 4-2 which suggest preferences for selecting source apportionment methods based on the time frame of the problem, the ambient data base and the filter media (Pace, 1983). The availability of source mass emissions or chemistry data may be limited by whether it is possible to test the source or to predict the timing or consistency of its operation.

4.1.3 Nature of the Problem

The complexity of the problem, (that is, whether it involves many suspected sources or a single likely source), influences the selection of methods. In a simple situation, some of the less quantitative or screening

TABLE 4-1

PREFERRED APPROACHES FOR SOURCE APPORTIONMENT (Pace, 1983)

		Ambient Data Base Available	
		TSP*	PM_{10}
Time Scale of the Nonattainment Problem	Annual	(a) applicable dispersion model corroborated by SEM or optical microscopy (b) applicable dispersion model	(a) applicable dispersion and receptor model (b) applicable dispersion model (c) receptor methods (at least two)
	24-hour	(a) applicable dispersion model corroborated by SEM or optical microscopy (b) applicable dispersion model	(a) receptor and applicable disperson model (b) receptor methods (at least two) (c) applicable dispersion model

Assumptions

* 1. TSP is collected on glass fiber filters, other filter media may be more suitable for receptor modeling.

2. Short-term emission inventories are difficult to obtain because of the nature of the source.

TABLE 4-2

APPROPRIATE FILTER MEDIA FOR USE WITH RECEPTOR MODEL STUDIES (Pace, 1983)

Laboratory Technique	Filter Type			
	Glass Fiber	Quartz Fiber	Polycarbonate	Fluorocarbon
Elemental Analysis (Mass Balance) (Factor Analysis)	3	2	1	1
Optical Microscopy	2	2	2	2
Automated SEM	2	2	1	2
Carbon	2	1	3	3

1. Recommended
2. Useful under some circumstances or to some analysts
3. Not recommended

methods may be adequate. In such cases, combinations of some of the simpler dispersion models, such as the PT series, or PAL, with receptor models such as optical microscopy, tracer methods, or spatial or temporal correlations, may suffice. Multiple sources may require the more refined dispersion models such as MPTER, RAM or ISC along with chemical mass balance or multivariate receptor methods.

The spatial extent of the problem affects the size and type of emissions inventory needed. If the problem is largely transport the applicability of the available models may be limited.

The nature and chemistry of the emissions of the suspected sources is important for several reasons. Some sources are precursors of secondary particulate matter such as sulfates. Determining the sources of these sulfates generally requires a dispersion model that accounts for chemical transformations. In may cases, particularly in the eastern United States, regional scale models would be needed. The chemistry of the emissions of each source or source category must be sufficiently different to enable the chemical mass balance and the multivariate methods to distinguish among them. Sources that are chemically very similar cannot generally be distinguished using these methods.

The size range of the emissions of the suspected sources affects method selection. Sources that emit primarily large particles include the "fugitive dust" sources such as windblown or mechanically generated or resuspended dusts. Large particles are amenable to analysis by optical or scanning electron microscopy or x-ray diffraction but, if they come from a variety of soil or crustal related sources, their specific sources are difficult to distinguish by chemical methods. Fine particles, generally defined to include those smaller than 2.5 µm, are usually associated with combustion sources.

They are too small for optical microscopy and, in many cases, they are primarily carbon. In that case, they can only be distinguished by the chemical methods if they have a unique tracer such as lead in gasoline or vanadium in fuel oil. Fossil (as in fuel oil or diesel fuel) and contemporary (as in wood smoke or vegetative burning) sources of carbon can be distinguished to some extent by carbon dating chemistry (Stevens and Pace, 1984).

4.1.4 Complementary Methods

The complementary use of models can involve the use of two or more receptor models or the use of a combination of receptor and source/dispersion models. Table 4-3 shows the models best suited to complementary uses. The models most suited to complementary uses are those that operate on different data bases, algorithms and assumptions such that source contribution estimates are obtained independently.

In viewing Table 4-3, receptor methods may be thought of as three distinct groups of methods that represent, conceptually, three distinct perspectives on source contributions. The first of these groups, the qualitative methods, generally rely on ambient mass concentrations, often in conjunction with meteorological data. The second and third groups are listed as quantitative methods in the table. Group 2 includes mass balance (MB), factor analysis (FA), Target Transformation Factor Analysis (TTFA), multiple linear regression (MLR), and use of tracers. These Group 2 methods all rely on chemical features of the sources and the bulk ambient samples. In contrast, Group 3, consisting of optical microscopy (OM), scanning electron microscopy (SEM) and X-ray diffraction (XRD) relies on interpretation of chemical and physical

TABLE 4-3

MATRIX OF COMPLEMENTARY USES OF RECEPTOR AND SOURCE (DISPERSION) MODELS

	Receptor Models												Source (Dispersion) Models						
	Qualitative				Quantitative								Screening			Refined			
	Back-ground	Data Distr.	Time Corr.	Space Corr.	MB	FA	TTFA	OM	SEM	XRD	MLR	Tracers	PTMAX, PTDIS, PTPLU	PTMTP, PAL	Valley	CRSTER, MPTER, RAM, etc.	ISCST	AQDM, CDM, etc.	ISCLT
Receptor Models:																			
Qualitative																			
Background concentrations																			
Data distributions (lognormality, frequency)	C																		
Temporal correlations (yearly, monthly, weekend, daily, precip. events)	B	B																	
Spatial correlations (episodes, mapping, trajectories, cones)	A	B	B																
Quantitative																			
Mass balance (MB)	A	C	B	A															
Factor analysis (FA)	A	C	B	B	A														
Target transformation factor analysis (TTFA)	A	C	B	B	C	C													
Optical microscopy (OM)	A	C	B	A	A	A	A												
Scanning electron microscopy (SEM)	A	C	B	A	A	A	A	B											
X-ray Diffraction (XRD)	A	C	B	A	A	A	A	B	B										
Multiple Linear regression (MLR)	A	C	B	B	C	A	C	A	A	A									
Tracers	A	C	B	A	C	A	C	A	A	A	C								
Source (Dispersion) Models:																			
Screening																			
PTMAX, PTDIS, PTPLU	A	B	B	B	A	B	B	A	A	A	B	B							
PTMTP, PAL	A	B	B	B	A	B	B	A	A	A	B	B	B						
Valley	A	B	B	B	A	B	B	A	A	A	B	B	B	C					
Refined																			
CRSTER, MPTER, RAM, etc.	A	B	B	A	A	B	B	A	A	A	B	B	A	C	B				
ISCST	A	B	B	A	A	B	B	A	A	A	B	B	A	C	B	C			
AQDM, CDM, etc.	A	B	B	A	A	B	B	A	A	A	B	B	B	C	B	C	C		
ISCLT	A	B	B	A	A	B	B	A	A	A	B	B	B	C	B	C	C	C	

Key:

A = Usually complementary, generally provides new insight.
B = Sometimes complementary, may provide new insight.
C = Seldom complementary, may be redundant.

features of discrete particles found on the samples. Dispersion modeling provides yet a fourth group, or perspective, by virtue of its reliance on source emission rate estimates, meteorological data and dispersion parameters.

In general, the most complementary methods are those that are from differing groups, bringing differing perspectives to the analysis. Thus, methods within a group are usually most effectively used in conjunction with methods from a second group and not with other methods from the same group. Perhaps the most noteworthy is the combined use of dispersion models with any of the other three groups.

The following is a further discussion of the complementary aspects of selected features found in Table 4-3:

4.1.4.1 Background

A background determination complements and is even essential to almost any source apportionment study. It is useful in identifying particles of natural origin that are not subject to control; but also, it helps estimate the relative contributions of local influences as compared to the long range transport component.

4.1.4.2 Data Distributions

Analyses such as investigations of lognormality and frequency distributions are not particularly useful for source apportionment by receptor modeling, although they are needed to determine the representativeness of the days being modeled. This analysis may be useful for dispersion modeling where hypothetical meteorological conditions are used and the representativeness of these conditions vis-a-vis measured values needs to be determined.

4.1.4.3 Time Correlations

Time correlations give some preliminary insights into a problem. They are essential if the suspected source operates intermittently and changing meteorology can be easily accounted for, but in most cases the meteorology confounds a time series analysis such that temporal differences in concentration cannot be attributed to sources by time series alone. More elaborate statistical analyses such as multiple linear regression are usually needed.

4.1.4.4 Spatial Correlations

In this discussion, "spatial correlations" include correlations with wind direction and trajectories, as well as observed differences or simulations concerning sites measuring particulate matter. Spatial correlations are usually more useful than temporal analyses for particulate matter because the localized nature of many particulate matter sources lends itself to spatial comparisons. Such analyses may be particularly useful in conjunction with 24-hour analyses such as mass balance, microscopic methods and tracer analyses when their results are classified or grouped by wind direction. Spatial correlations are a reasonably effective supplement to dispersion modeling. For example, pollution roses can be used to check the reasonableness of source contributions determined by dispersion models and trajectory analyses can provide valuable insights into background contributions which are unaccounted for by dispersion models.

4.1.4.6 Mass Balance

Mass balance is generally appropriate and useful with any other method, but is especially useful with dispersion models. Methods such as factor analysis, multiple linear regression and tracers are often done as a preliminary step before doing a mass balance. These techniques may be useful in selecting which sources and fitting elements to consider in the mass balance approach.

4.1.4.7 Factor Analysis

Factor analysis provides information on which groups of aerosol features (elements, etc.) vary together; these groups can be interpreted as source categories. Thus, FA is moderately useful in determining if dispersion models have "missed" a major source category. Factor analysis is useful with other receptor techniques because it provides insight into source fingerprints. This information is vital to MB and MLR and helpful to microscopic studies. Target Transformation Factor Analysis is a form of factor analysis, thus it is redundant with that method.

4.1.4.8 Target Transformation Factor Analysis

TTFA is a combination of MB and FA and thus is redundant with these methods. It is useful as a complement to the microscopic methods, just as FA, MB, or MLR alone would be.

4.1.4.9 Optical Microscopy/Scanning Electron Microscopy

Polarizing light or optical microscopy (OM) is a semi-quantitative method which is very useful for identifying particles of natural origin such as pollens. It is very useful to corroborate such methods as spatial correlations, multiple regression, mass balance, factor analysis and dispersion models. It is also helpful to use automated scanning electron microscopy (ASEM) in conjunction with optical microscopy to formulate a quantitative assessment of source contributions.

4.1.4.10 X-Ray Diffraction

This method is particularly useful for identifying specific crystalline structures in soils and thus, is most useful when soil has been identified as a major source component but the methods used, (e.g., mass balance or the multivariate methods) cannot provide more specific information on sources. The x-ray diffraction analysis can only help when the suspected soil sources have differing minerology or crystalline structure.

4.1.4.11 Multiple Linear Regression

MLR is particularly useful with optical and scanning electron microscopy because it relies on different information or features of the ambient sample. It is also used to help quantify the contributions of source groups identified by factor analysis. It is usually redundant with mass balance, TTFA and tracer methods. It is most useful when chemical composition data for a large number of observations are available.

4.1.4.12 Dispersion Models

The dispersion models generally require an analysis of background concentrations because as much as half or more of ambient particulate matter in an urban area may originate from beyond the local airshed and thus would not be included in the model. Dispersion models in general are complemented by receptor methods, especially microscopy and mass balance analysis. This is because receptor methods bring an entirely different perspective to the analysis and rely on different information and assumptions. They are especially useful to identify uninventoried or misinventoried sources or source categories. The microscopic methods are a useful complement to screening or refined models and are also helpful to corroborate the refined dispersion models. The screening models such as the PT series are useful preliminaries to a refined model analysis.

4.1.5 Resources

No discussion of method selection would be complete without a discussion of resource considerations. The selection of methods is affected in some part by the expertise and experience of the staff in the various methods, as well as their availability. Equally important is the availability of funds to purchase consulting or contract assistance. The time available to come up with an answer may also preclude certain types of analyses, particularly those that require data gathering.

One way of conceptually structuring a study design so that time, personnel and available funds are considered is the three level approach (Stevens and Pace, 1984). The three levels are not "cookbook" recipes since all of the ingredients (methods) and their amounts (resource requirements), etc., are not firmly fixed. The three levels are intended as rough guides, or benchmarks, and are flexible to accommodate the wide range of real world situations and constraints that are likely to be encountered. Within each level, the time frame and nature of the problem, the existing data base, the applicability of complementary methods and the available resources must be considered.

4.2 A Three Level Approach

Level I uses existing data or data that can be readily obtained from analyses of existing samples. The models used are those that apply to the data set and that do not require extensive resources for their computation. In Level I, basic analyses are used to identify contributing sources and, if possible, obviate the need for further analyses. Otherwise, the Level I analyses will serve to narrow down the areas to be studied in more detail in Level II. Some source-types can be eliminated from further consideration after Level I is finished, thereby focusing data gathering efforts in Level II. Combinations of source and receptor models can be used in this process. If the sources contributing to the high concentrations of particulate matter are apparent and sufficiently certain, no further work will be needed beyond Level I.

Level II encompasses more refined analyses than the first, including performing additional analyses on existing samples, acquiring new samples from existing monitoring networks and a limited amount of new sampling. Such new sampling could be used to obtain component "fingerprints" for source emissions (e.g., road surface loadings and silt content) or selected ambient samples. Level II uses models that require more detailed inputs and larger computational facilities. However, models and analytical methods are of a standard nature. Combinations of methods can be used.

Level III involves the acquisition of new data from new sampling activities and programs. These programs can be quite extensive, e.g., the deployment of a special monitoring network in order to obtain a year's worth of particle size-segregated samples suitable for detailed chemical characterization. Analysis procedures can incorporate a variety of models with very detailed inputs. Models and analytical methods may be of a nonstandard nature, i.e., developed exclusively for the project.

Suggested approaches to these three levels are described in the following subsections. The suggestions and recommendations made are not rigid prescriptions but are simply meant to convey the levels of analysis that may be required, based on the collective experience of the authors.

4.3 Level I: Gathering, Evaluating, and Using Existing Data with Simple Models

The objective of a Level I study is to determine the likely causes of a given pollution problem with only a modest investment of time and resources. In a Level I study, existing data and simple analyses are used to obtain answers to questions pertaining to source/receptor (source/monitor) relationships. A Level I study does not involve collecting any new data through new monitoring programs. The first step in such a study is to gather the existing data, the second is to evaluate the data, and the third is to determine if additional data are needed and are feasible to obtain. Needed for these analyses are source, meteorological, and ambient data. The collection, compilation, and review of these data are discussed first below, followed by suggested analysis procedures. While a Level I study may, in some cases, (e.g., where the culpable source is isolated and easily defined,) be adequate for control strategy development, in most cases, a Level I study will serve as the basis for defining the scope and nature of a Level II or Level III study.

4.3.1 Source Data

Various types of source data can be used in a Level I analysis. Such data include emission rates by total mass or particle size, composition, and variability with time, and source configuration parameters (location, height, flow rate, temperature, etc.). These data are discussed in Section 3.2.

The available data should be organized and reviewed to identify likely important contributors to the ambient pollutant levels. An overview of the major source-to-monitor alignments and initial insight into the likely important contributors to the measured pollutant concentrations can be obtained if the major point sources are plotted on a map of the study area. Additional information on likely contributing sources can be gained by gathering and reviewing the SLAMS and NAMS site surveys (U.S. EPA, 1979b) and data from any previously developed microinventories for the area(s) surrounding (within a radius of 2 km) the monitor(s). If SLAMS and NAMS site surveys do not exist, such surveys can be performed with minimal effort for sites of critical concern in a Level I study, or they can be delayed until it is determined whether a Level II analysis is needed.

The source emissions data should next be organized and compiled. Compilations by source-type categories (e.g., power plant, steel plant, municipal incinerator, traffic-related), with the emission rates in each category summed and then sorted by the category emission totals are recommended. These source groupings can then be maintained through subsequent dispersion modeling analyses (e.g., ISC) and also used for comparison to measured concentrations (by particle composition, if available). If particle composition data for the source emissions (chemical species, particle sizes, etc.) are available, they could also be tabulated for each source, starting with categories of highest emission rates. From these tables, chemical species unique to specific sources (i.e., tracers), and the dominant chemical species and particle sizes in the study area can be identified.

4.3.2 Meteorological Data

All readily available meteorological data should be collected and evaluated for validity and representativeness to the study area. Possible sources and evaluation procedures for meteorological data are described in Sections 2.3.7 and 3.3. Once a valid, representative meteorological data set has been assembled, it is recommended that the locations of all the wind measurement stations be noted on the same map with the major point sources and that 24-hour vector average wind speeds and directions be generated for the days of interest. Vector averages at each station for a given day can then be plotted at each of the meteorological station locations. Once the wind vectors have been plotted, the daily wind fields can be analyzed for dominant directional patterns and any anomalous wind directions due to channeling effects. Other suggested evaluations of meteorological data include comparing tall tower data (if available) with surface level data (to estimate any change of direction with height) and comparing local flow patterns with the overall synoptic pattern apparent from NWS surface weather maps (to assess long-range transport).

4.3.3 Ambient Data

Measured ambient pollutant data should be gathered from all existing monitoring networks. Historically, most particulate matter monitoring has involved hi-vol samplers which collect TSP data. More recently, some sampling has been conducted using dichotomous, size-selective hi-vol or other samplers hich collect PM_{10} data. Most Level I studies will involve the analysis of TSP data. Depending on the analyses performed, such studies may also provide information regarding source contributions to PM_{10} concentrations. Potentially helpful data bases are described in Section 3.4. In order to assess the source-to-monitor relationships, the locations of the monitors can be plotted on the same map as the source and meteorological data.

4.3.4 Procedures (Level I)

A Level I modeling study involves performing a series of relatively simple, straightforward analyses designed to enable the analyst to deduce cause and effect relationships between source emissions and ambient concentrations. Each analysis can provide information to make it possible to eliminate insignificant sources and focus in on important contributors. Work performed by Brookman (U.S. EPA, 1983d), and summarized in Section 5.2, provides a good example of a basic Level I study approach. Additional protocol information is contained in the study report.

4.3.4.1 Qualitative Receptor Modeling Analyses

A good place to start conducting a source apportionment study is with the qualitative receptor modeling analyses described in Section 2.3.7. These analyses can be performed readily using total particulate matter concentrations, and, if data are available, they can also be performed using constituent and size-segregated concentrations. The results of such analyses must be interpreted with due consideration of the sampling instruments, filter media, and other factors involved in the collection of the particulate matter samples, as discussed in Section 3.4. An appropriate initial analysis for a Level I receptor modeling study is the determination of background concentrations. By conventional definition, background concentrations are those caused primarily by sources located outside the study area. Background concentrations can be developed for both long-term (annual, seasonal, and monthly) and short-term ($\leq$ 24 hour) periods for the various particulate matter concentrations. Several years of data can be combined to obtain sufficient samples for short-term and monthly averages.

The next analysis of interest is the trend analysis in which annual mean ambient concentrations, less the corresponding annual background concentrations, are plotted as a function of time (for as many years of data as are available). The results can then be compared to yearly emissions data (if available) to see if there is any agreement between changes in ambient levels and events such as source shutdowns, source startups or implemented control strategies. A correspondence (i.e., 1:1) between percentage changes in total emissions versus percentage changes in total ambient levels (less background) is supportive of the accuracy of the emissions inventory. Poor agreement may be indicative of deficiencies in the inventory. If no trend emerges, it may be possible to obtain some trend information if the individual daily concentrations are first grouped according to recurring patterns of synoptic (i.e., air mass) scale meteorological conditions. When these averages are plotted, trends may become evident for certain wind directions relevant to specific source-to-monitor alignment directions.

Next, more detailed temporal and spatial correlation analyses can be performed. These include seasonal and monthly trend analyses, weekday/weekend analyses, wet/dry day analyses, episode day analyses and spatial mapping. Seasonal and monthly trend analyses can be used to identify traffic, agricultural, and other fugitive dust influences. Weekday/weekend analyses can also help identify traffic-related impacts. Wet/dry day analyses can provide an initial estimate of the magnitude of the total non-traditional fugitive particulate matter impacts. Episode day analyses are useful for separating local from distant source contributions. Spatial mapping can be used to show source contribution patterns for various time periods (annual, wet/dry days, episode days, persistent wind days, etc.), with comparisons from one time period to another revealing the relative magnitude of various source category influences.

Correlation coefficients and time series analyses can also be used to relate receptor concentrations to sources. Analyses performed on particulate matter data for multiple sites can be used to identify sites and periods influenced by local sources. Analyses performed on particulate matter data and other parameters can be used to help reveal the location and relative influence of the nearby sources. Also suitable for further study are those cases where concentrations at all sites rise simultaneously (i.e., episode days).

If the wind direction was persistent on the sampling days of interest, pollution roses can be of value in determining contributing sources, especially if chemical composition data are available. If the bulges in the pollution rose concentrations at multiple sites point toward the same location, triangulation may help pinpoint specific sources.

4.3.4.2 Dispersion Modeling Screening Analyses

For the sampling sites of concern, screening source/dispersion modeling analyses can provide information concerning source contributions based on the inventories of source data obtained for each site. Various models can be used for this purpose depending on the objective of the analysis, the type of sources in the area and the availability of computational resources. The primary objective of a screening dispersion modeling analysis is to eliminate insignificant sources from further consideration. Dispersion modeling to meet this objective is discussed below. This screening dispersion modeling will also provide information on the relative magnitude of source contributions and thus help focus the direction of subsequent analyses. Dispersion modeling techniques designed to better quantify source contributions are discussed in Section 4.4 (Level II).

If possible, the model selected for a screening analysis should have the capability to 1) predict individual source contributions at user-defined discrete receptor points (i.e., the monitoring sites of concern), 2) determine contributions from multiple sources, 3) accept user-defined meteorological data, 4) account for particle settling (pollutant deposition), and 5) predict contributions from point, area, volume (i.e., certain elevated area), and line sources. Ideally, the model should also be able to directly determine contributions for the time period(s) of concern and be able to reliably calculate impacts in locations with complex terrain. Since receptor modeling analyses are generally concerned with particulate matter collected on filters during short-term (1-24 hour) time periods, discussion of screening dispersion modeling analyses in this subsection is limited to these short-term time periods. A comprehensive evaluation of the capabilities of some dispersion models, for use in receptor modeling applications, is shown in Table 4-4. The model capabilities ratings in Table 4-4 provide a useful measure of model features, but when models are selected for use in specific situations EPA guidance (U.S. EPA, 1978a) should also be considered. See Section 2.2.2 and the respective model user's guides for additional discussion of the capabilities of these dispersion models.

If computer resources are not available, rough estimates of the potential magnitude of the source contributions can be obtained using published nomographs or by performing hand calculations following procedures described by Turner (1970) or the Guidelines for Air Quality Maintenance Planning and Analysis Volume 10R (U.S. EPA 1977a). If limited computer resources are available, such estimates can be obtained using the EPA UNAMAP models PTMAX, PTDIS, or PTPLU, but all three of these models are designed for point sources only. PTMAX and PTPLU will not predict source contributions at user-defined receptor locations. The above methodologies can be used to eliminate insignificant sources from further consideration, but are generally inadequate for estimating the combined contributions of multiple sources. Furthermore, none of the methodologies have the capability to account for particle deposition.

TABLE 4-4

SOURCE (DISPERSION) MODEL CAPABILITIES RATINGS

Model Input/Options	PTMAX	PTPLU	PTDIS	PTMTP	PAL	CRSTER	TEM-8	MPTER	COMPLEX-I	COMPLEX-II	RAM	ISCST	VALLEY	AQDM	TCM-2	CDMQC	ISCLT
Source Information (See Key 1)																	
All Sources																	
Location coordinates				2	2	1	2	2	2	2	2	2	2	2	2	2	2
Ground elev. above sea level						1		2	2	2		2	2				2
Emission rate	1	1	1	2	2	1	2	2	2	2	2	2	2	2	2	2	2
Particle removal by exp. decay							2	2	2	2	2	2	2		2	2	2
Part. size (deposition) para.*												5					5
Emission rate variability**					2	1		2	2	2	2	2				2	2
Point Sources																	
Stack height	1	1	1	2	2	1	2	2	2	2	2	2	2	2	2	2	2
Stack exit velocity	1	1	1	2	2	1	2	2	2	2	2	2	2	2	2	2	2
Stack exit diameter	1	1	1	2	2	1	2	2	2	2	2	2	2	2	2	2	2
Stack exit temperature	1	1	1	2	2	1	2	2	2	2	2	2	2	2	2	2	2
Adjacent building dimensions***												3					3
Area, Volume, and Line Sources																	
Effective emission height					3		3				3	3	3	3		3	3
Source dimensions					3		3				3	3	3	3	3	3	3
Receptor Information (See Key 2)																	
Location coordinates			1	5	5	1	1	5	5	5	5	5	1	5	1	5	5
Elevation above sea level						1		5	5	5		5	1				5
Elevation above ground				5	5			5	5	5	5						
Meteorological Information (See Key 3)																	
Wind direction				5	5	4	5	5	5	5	5	5	3	3	3	3	3
Wind speed	1	1	1	5	5	4	5	5	5	5	5	5	3	3	3	3	3
Atmospheric stability	1	1	1	5	5	4	5	5	5	5	5	5	3	3	3	3	3
Temperature	1	1	1	5	5	4	5	5	5	5	5	5	2	2	2	2	2
Mixing height		1	1	5	5	4	5	5	5	5	5	5	2	2		2	2
Wind speed varia. with height		1			5	4	5	5	5	5	5	5	2		2	2	2

TABLE 4-4 (Continued)

SOURCE (DISPERSION) MODEL CAPABILITIES RATINGS

Model Input/Options	PTMAX	PTPLU	PTDIS	PTMTP	PAL	CRSTER	TEM-8	MPTER	COMPLEX-I	COMPLEX-II	RAM	ISCST	VALLEY	AQDM	TCM-2	CDMQC	ISCLT
Rural/Urban Considerations (See Key 4)																	
Stability classifications	3	3	3	3	3	1	3	1	1	1	3	3	3	2	3	2	3
Dispersion coefficients	1	1	1	1	1	1	1	1	1	1	3	1	1	1	1	1	1
Other Attributes (See Keys)																	
Direct output of 24-hour avgs. (Key 5)				2	2	2	2	2	2	2	2	2	1	1	1	1	1
Complex terrain (Key 6)				1		1		1	2	2	1	1	2				1
Source contribution listings (Key 7)				2	1		1	2	2	2	2	2		1	1	2	2
TOTAL CAPABILITIES RATING	12	14	14	56	67	39	58	70	71	71	73	81	46	41	37	48	65

*   = Mass distribution of particle sizes, gravitational settling velocities and surface reflection coefficients
** = As a function of time or meteorology
*** = Height, length, width

Key 1:
1=Single source (location)
2=Multiple sources (locations)
3=Multiple sources, improved capability
5=Multiple sources, superior capability

Key 2:
1=Polar or Cartesian grid only
5=Discrete locations

Key 3:
1=Built-in or single hourly values only
2=Applies to stability wind rose time period
3=Stability wind rose (STAR) format
4=Hourly, CRSTER preprocessed data only
5=Hourly, preprocessed or user-defined data

Key 4:
1=Rural
2=Urban
3=Either

Key 5:
1=From 24-hour STAR input
2=From hourly averages

Key 6:
1=Up to stack height only
2=Any height

Key 7:
1=Some sources;
2=Most sources

A simple computerized screening model for multiple point sources is the EPA UNAMAP model PTMTP. With PTMTP, the user can define the receptor points, input the meteorological data of interest, and specify the time periods to be modeled. Alternatively, if area and line sources are expected to be important, the EPA point, area and line (PAL) source model can be used for screening modeling analyses. Unfortunately, neither PTMTP nor PAL can account for particle deposition, a serious deficiency for analyses of monitors significantly impacted by fugitive dust sources.

If sufficient computer resources (core space and data storage) are available, the EPA MPTER and RAM models offer some additional valuable capabilities for use in screening modeling analyses. MPTER is designed for rural point sources only. RAM should be used for urban point and area sources. These models are designed for use in more comprehensive dispersion modeling analyses, but, with appropriate input data, MPTER and RAM can be used in a screening analysis mode. MPTER and RAM can be used to calculate particle deposition, but only through the use of an exponential decay term.

If the computer resources and required input data are available, the EPA ISCST model is probably the best available for use in screening modeling analyses in relation to receptor modeling applications. In addition to the capabilities of the models discussed above, ISCST can predict contributions from point, area, and volume sources and directly account for particle settling by particle size. Like MPTER and RAM, ISCST is designed for use in refined dispersion modeling analyses, but can be operated in a screening analysis mode when appropriate data are used as input.

All of the aforementioned models are short-term models designed to use hourly meteorological data to calculate hourly impacts which are then averaged or otherwise applied to 24-hour periods. As an alternative, for screening dispersion modeling analysis purposes, 24-hour impacts can be determined using dels designed to calculate long-term (i.e., monthly, seasonal, or annual) erage impacts. For such analyses, artificial or hypothetical meteorological put data must be constructed to simulate conditions that occur over 24-hour riods. Of the models of this type shown in Table 4-4, only AQDM, CDMQC, and CLT can be used to predict source contributions at discrete user-defined ceptor points. Only ISCLT accounts for particle deposition.

None of these models is specifically designed for screening analyses for e 24-hour impacts of multiple sources. Screening dispersion modeling alyses can proceed at different levels of detail. The choice of the level detail employed and the model selected for a given situation will depend on number of factors including 1) the objective of the analysis, 2) model and put data availability and compatibility and 3) the desired precision of sults. Simplifying assumptions must be made in screening modeling alyses. The initial simplifying assumptions are those contained within the mputational algorithms of the various models. Additional simplifying sumptions are made in 1) the choice of a model, 2) the selection of model tions and 3) the treatment of model input data. Thus, screening modeling alyses inherently involve making trade-offs between the reliability and the ficiency of the analysis.

The following screening dispersion modeling approaches are suggested to et the objective of identifying insignificant sources. These approaches are tended only as starting points for other ideas since many workable proaches are possible. For a given analysis, the specific procedures used st be tailored to the individual situation encountered.

Insignificant point sources can be identified with reasonable reliability d efficiency using the PTDIS model. PTDIS calculates 1-hour impacts based on a user-specified array of wind speed and atmospheric stability combinations, regardless of wind direction. An array of applicable wind speed/stability combinations is provided in Table 4-5. With PTDIS, each source must be modeled separately with the source-to-receptor (i.e., source-to-monitoring site) distance specified. To ensure that no potential impacts are overlooked, a few closer and more distant receptors should also be modeled. Each source should be modeled using simplifying assumptions that maximize the modeled impacts. Thus, point sources are modeled at maximum emission rates, assuming no particle deposition. Sources with insignificant 24-hour impacts are identified as those that PTDIS shows have insignificant 1-hour impacts. Since the modeled contributions of all the modeled sources will tend to be overpredicted, no potentially significant sources will be overlooked.

TABLE 4-5

APPROPRIATE COMBINATIONS OF WIND SPEED AND STABILITY FOR USE IN PTDIS SCREENING MODELING ANALYSES

Pasquill-Gifford Atmospheric Stability Classifications	Wind Speeds (m/s)
A	1 to 3
B	1 to 5
C	1 to 5, 7, 9, 12, 15
D	1 to 5, 7, 9, 12, 15, 20
E	1 to 5
F	1 to 3

Insignificant area, volume, (i.e., elevated area) and line sources can be identified using the following two equations. In order to use these equations, all area, volume and line sources must be treated as square area sources. The first thing to be determined is whether the monitor in question is located within or "near" the area source. For the purposes of this screening analysis, "near" is defined as within a factor of 0.6 Δx + 100 meters of the center of the area source, where Δx is the length of the side of the area source. Equation 1 applies to monitors located within 0.6 Δx + 100 meters of the area source center and equation 2 applies to more distant monitors

$$Q_I = \frac{C_I \bullet (\Delta x)^{1.75} \bullet u}{18 \bullet 10^6} \qquad \text{Equation 1}$$

$$Q_I = \frac{C_I \bullet (\Delta x)^{1.5} \bullet u}{18 \bullet 10^5} \qquad \text{Equation 2}$$

where:

Q_I = an emission rate in g/s
C_I = an impact in μg/m³
Δx = the length of the area source side in m
u = a wind speed in m/s

Equation 1 was obtained from the U.S. EPA Guidelines for Air Quality Maintenance Planning and Analysis Volume 10R (1977a) and equation 2 was derived empirically using the ISCST model.

If a 1-hour concentration of 10 μg/m³, (roughly equivalent to 24-hour concentrations of 5 μ/m³, see Volume 10 above) is assumed to be insignificant sources as those with a $Q/(\Delta x)^{1.75}$ ratio of less than 5.56×10^{-7} and equation 2 identifies insignificant sources as those with a $Q/(\Delta x)^{1.5}$ ratio of less than 5.56×10^{-6}. Since the above procedures are designed to overpredict contributions, sources whose impacts are deemed insignificant can be eliminated from further consideration.

4.3.4.3 Qualitative and Quantitative Receptor Modeling Analyses

Very often additional measurements taken on filter samples may be available. Several State and local agencies perform routine chemical analysis of selected filters for certain chemical species. Others submit a certain number to microscopic analyses. As mentioned in Section 3.4, EPA has been collecting size and chemically resolved samples at IPN sites in many major U.S. cities (Watson, et al., 1981). These data can be used in additional Level I analyses to verify the conclusions drawn from previous analyses. The data quality issues discussed in Section 3.4 should be taken into consideration when these data are analyzed.

Time series plots, pollution roses, and spatial mapping of chemical species such as lead and bromine (which are almost always indicative of auto exhaust contributions) and aluminum and silicon (which are usually contributed by soil dust) can reveal source contributions which might not be evident when only mass measurements are used.

Rudimentary mass balances can be performed to determine the relative contributions of various source categories. For example, assume that approximately 8 percent of soil is aluminum and that 8 percent of the aggregate auto exhaust emissions are lead. By dividing aluminum and lead concentrations by 0.08, one achieves a rough estimate of the soil and auto exhaust contributions to a mass concentration. One could choose a lower limit of these compositions, e.g. 5 percent, and could achieve a very conservative approximation of these sources' contributions. If they are still minor contributors, they could be removed from further consideration for control. A review of the source compositions in Appendix B for sources suspected as a result of analyses performed on total particulate matter data would allow this procedure to be applied to a number of sources, if their key chemical species were measured.

Microscopic analyses are most informative when three conditions are satisfied: spatial and time series plots should show individual sites or "hot spots" with high concentrations; pollution roses should show a directional tendency; and alignment of the monitor(s) and the major sources in the emissions inventory should show correspondence with the prevailing wind direction. Though it requires a skilled microscopist to perform semi-quantitative analyses of filter samples, a qualitative examination of the majority of the particles observed on an ambient filter, in comparison to those observed on sieved samples taken from suspected sources, can be revealing. Samples can be taken, dried, sieved and mounted on slides in 1.518 index of refraction immersion oil for examination. Several portions of a hi-vol filter can also be immersed in an oil of 1.518 index of refraction (this makes the filter disappear under transmitted light). If the filter deposit is dominated by the source material, it is probably a major contributor. If absolutely none is found, then other sources must be sought. If the deposit shows a mixture of materials, more complete microscopic analysis by an expert will be required.

Probably the most important step of a Level I assessment is the evaluation of the extent to which the existing data support a control action. In many cases, particularly those of an exceedance of standards at a solitary site, the conclusions drawn from the varied uses of existing data described here will be sufficient to identify major contributing sources and devise a strategy to control them.

Even if this is not possible, the Level I examination will result in conclusions about which existing sources are not major contributors, thereby narrowing the list of those which must be dealt with in greater detail in a Level II strategy.

4.3.5 Resources

Assuming that existing data have been acquired and validated (a task which can take from one man-week to one man-year, depending on the specific situation) the analyses described here should not result in more than several man-months of effort. Computational capability requirements are minimal, though a hand calculator or personal computer with spreadsheet and graphics software would greatly facilitate the work. The analyses discussed here can be performed with little or no need for additional monitoring and with a minimal number of laboratory analyses. The cost of studies of this magnitude should range from $5,000 to $25,000.

4.4 Level II: Acquire More Data without Extensive Sampling and Use More of the Capabilities in Refined Models

The cause and effect relationships between source emissions and ambient concentrations can often be deduced using analyses performed at the level of sophistication described in the preceding section (Level I). However, while the answers might be obvious as to which sources are primarily responsible for a given air pollution problem, a quantitative apportionment of that responsibility may be impossible or may lack a reasonable degree of certainty and thus be insufficient to justify the formulation and implementation of expensive emission control strategies. If this proves to be the case, a more rigorous study, of the type discussed in this section (Level II), can be performed.

4.4.1 Source Data

The emission inventories for the sources that are considered to be the most likely contributors to the problem (on the basis of the Level I analyses) should be checked and verified or corrected. This process could start with the 5 to 10 most likely contributors and, if need be, proceed to other sources based on a prioritization scheme starting with the largest and nearest sources. Parameters of concern include material throughputs, control efficiencies, stack heights, stack diameters, exhaust gas flow rates, exhaust gas temperatures, etc. Emission rates can be checked by comparing inventoried values to new values calculated using the best available current emission factors. If emission rates vary greatly from day to day, hour to hour or over other relevant time periods, it would be valuable to calculate such short-term emission rates for inclusion in the inventory.

Sources such as road dust, storage piles, open burning, playground dust, etc. are often important contributors to particulate matter problems. If these types of emissions were not evaluated in the Level I analyses, or if they were included on a broad spatial scale only, then it would now be advisable to compile these emissions using microinventory techniques around each sampling site. Comprehensive microinventories may not be required in all cases, but they are usually of value, especially at receptor sites suspected of being influenced by nearby sources of fugitive dust. The procedures for developing microinventories are discussed in Section 3.2. Daily emission inventories may be needed if emission rates vary greatly from day to day, but they can be quite difficult to obtain.

Most existing inventories do not contain data on particle size or chemical constituents. Therefore, for a Level II analysis, it may be necessary to obtain source emission samples for physical and chemical analyses using inexpensive grab sampling techniques. Chow, et al., (1981) describe the following methodology for taking these samples:

> "Several common source types are amenable to "grab sampling", resuspension sampling and subsequent chemical analysis. These source types include: road dust, road salt, soil, storage pile contents, loading and unloading materials, and baghouse and cyclone residue.

> A representative sample of the material can be collected in a ziplock bag. In the laboratory it can be dried, sieved through a Tyler 400 mesh sieve (38 μm screen size) and resuspended for sampling with devices similar to those used to take ambient samples. The chemical analyses performed on these resuspensions should be the same as those of the ambient samples."

4.4.2 Meteorological Data

The desire to obtain better quantification of source contributions to ambient concentrations may result in the need for additional, or more representative, meteorological data than were used in the Level I analyses. In Level I, dispersion modeling analyses can be performed using representative hypothetical meteorological data (e.g. Table 4-5), and receptor modeling analyses can be performed using data obtained from published or other readily available historical records. In a Level II study, it may be necessary, or at least advisable, to construct a computerized data base of meteorological information for multiple years, parameters, and monitoring sites. Such a computerized data base could be used to calculate surface and upper air wind trajectories based on data obtained from multiple NWS or other monitoring sites.

The more refined dispersion models can use either hypothetical or actual meteorological data. The refined short-term models can calculate hourly, daily, or other short-term average impacts using up to a full year of hourly meteorological data. Such a large data set can be used efficiently only if it is computerized. If dispersion modeling is going to be performed on a large number of sampling days of data, then it is advisable to obtain computerized data sets of the hourly meteorological data. For NWS stations, such data sets can be obtained from the NCDC in the format required for input to the CRSTER preprocessor.

The representativeness of the meteorological data is of considerable importance to the Level II study. Proximity and similarity of location are the primary concerns as discussed in Section 3.3. The meteorological station(s) should be located reasonably close to the sources and sampling sites and in an area of similar topography. If no NWS stations meet these criteria, it may be possible to obtain wind data from a nearby non-NWS location and then merge these data with data for parameters other than wind obtained at the NWS site. Uncertainties should be assigned to each of the parameters measured. If the available meteorological data are deemed unrepresentative, a Level III study will be required to gather appropriate data.

4.4.3 Ambient Data

Level II analyses become necessary when the results of Level I analyses are inconclusive or incomplete. This will often occur because of a lack of existing data on the composition of the ambient particulate matter. It is often possible to obtain such data by analyzing the material on existing filters or by collecting a limited number of new filters. A suggested procedure for selecting filters for subsequent analysis (for particle size, chemical constituents, and other properties) follows.

For an "ideal" receptor modeling study, a large number of the available filters from a monitoring site would be subject to analysis and subsequent receptor model evaluation. Such an approach is not feasible when resources are limited and only a small subset of the available filters can be analyzed. It becomes necessary, therefore, to select filters which are representative of a wide range of conditions. When short-term particulate matter concentrations are of concern, the selection of filters for analysis can be limited to some of the days of high concentrations plus a few clean day filters for comparison. When long-term particulate matter concentrations are the problem a broader selection of filters is warranted. If both the long- and short-term time frames are of concern, a suggested approach is to select filters that, taken together, are reasonably representative of annual average conditions but that also include conditions where maximum short-term concentrations and source impacts occur.

The following criteria are suggested for use in the selection of the ambient sampling day filters to be analyzed:

- Select filters from day(s) with widespread high particulate matter concentrations (episode days). By selecting the date(s) on which most of the monitors indicated high concentrations, the primary causes of the particulate matter problem can be identified and studied.
- Select filters from day(s) with light and variable winds. Filters from such days would represent a homogeneous mix of contributions from various sources.
- Select filters from day(s) with "average" meteorological conditions. Filters from day(s) which have wind speeds and stabilities close to the average for the year are selected to be representative of days with typical contributions from each source.
- Select filters from day(s) with high wind speeds. Filters analyzed for such days will indicate the extent to which certain resuspended material and fugitive emissions affect the monitors. (Useful if windblown dust is suspected as a major source.)
- Select filters from day(s) with low particulate matter concentrations. Filters from those days having low particulate matter concentrations (non-precipitation days) are selected to be representative of days with minimal impacts from each source. (Useful if annual average concentrations are of interest.)
- Select filters from day(s) with persistent winds coming from the direction of sources previously identified as suspected contributors. Filters from such days can be used in direct comparisons to dispersion model results to evaluate the accuracy and representativeness of source emission rates and other source configuration parameters.

It is also advisable to analyze several typical "background" filters from monitors outside of the study area in order to obtain data on the composition of material coming into the study area.

If additional ambient sampling is necessary, important technical considerations include sampling locations and periods, sampler type, particle size, filter media and the sample preparation requirements of the particle analysis instruments (Gordon, et al., 1983). For a Level II analysis only a few samplers should be needed at locations where existing particle size and composition data are inadequate. Such sampling would probably best be performed with dichotomous samplers to obtain fine and coarse fractions on Teflon or Millipore filters to facilitate chemical and coarse microscopic analyses. Quartz filters could be used if sampling for carbon and ions is needed. The results from such sampling could then be used to judge the accuracy of existing particle composition data obtained from hi-vol sampling.

4.4.4 Procedures (Level II)

4.4.4.1 Receptor Modeling Analyses

Some idea of the most likely contributors to each receptor should have resulted from the Level I efforts and this can be used as guidance in choosing the further analyses of receptor samples. For these sources, the source characterization literature in Appendix B can be surveyed to 1) determine which chemical and physical properties will identify and help to quantify these sources, and 2) decide which analysis methods are appropriate for the existing samples.

Not all analyses can be performed on all filter media. For example, x-ray fluorescence (XRF) is inappropriate for samples taken on fiber filters because of the x-ray absorption in this thick filter media. XRF is very good for Teflon and other thin pure membrane filters. The blank levels of the filters must be much less than the concentrations of the species being measured. These levels can vary from batch to batch of filters, and if blank filters from the sampling batches have not been saved, erroneous results may be obtained. Many glass fiber filters contain organic binders which will hinder any analysis for carbonaceous species.

Watson, et al., (1981) discuss the effects of sulfate and nitrate artifact formation on filters and show how a change of filter media during a sampling program can yield an artificial increase in both total particulate matter and sulfate levels which might be interpreted as a sudden change in source contributions. The data interpretation efforts in Level II cannot be separated from the measurement process, and each additional analysis of existing samples must be thoroughly validated.

An important aspect of receptor modeling is the use and propagation of measurement precision to the model results. These precisions must be acquired with any additional analyses through routine replicate and blank analyses. Watson, et al., (1983) describe methods of using these analyses to obtain the precision of analysis results.

To quantify source contributions, a chemical mass balance calculation may be the most straightforward approach. This requires a source composition matrix in addition to ambient component concentrations.

If more than 50 receptor samples with chemical characterization measurements are available, then the multiple linear regression or factor analysis models can be used to narrow down the number of contributing sources and possibly to calculate source compositions.

A standard factor analysis can be performed using many standard statistical packages such as Statistical Package for the Social Sciences (SPSS), Biomedical Data Processing Programs (BMDP), and Statistical lications Systems (SAS). A standardized correlation matrix of all iables and a varimax rotation is the most commonly used configuration. The ber of dominant factors should correspond to the number of dominant rces, and the chemical species with which these factors are most highly related can be used with existing source composition information drawn from endix B to associate each factor with a source type.

If the source mix is such that fairly unique tracers can be identified h different sources, factor analysis will confirm this. Such a tracer will highly correlated with one factor but not correlated with any other nificant factor (Kleinman, 1977). The multiple linear regression (MLR) el can be applied using tracer species. The coefficients represent the erse of the tracer concentration in the source emissions, and the product each coefficient and the receptor concentration of the corresponding tracer ment yields the contribution of that source to the total mass concentration sured at the receptor. If the "effective variance" weighting (Watson, et , 1983) is used to perform the MLR least squares fit, then each measurement l be weighted in inverse proportion to its uncertainty and a realistic or bound will appear in the result.

If it appears that several sources are contributing substantial quantities the same chemical species, then a Target Transformation Factor Analysis FA) can be used to derive a source composition matrix. Hopke, et al., 83) have created the FANTASIA computer program which will perform this lysis and the subsequent mass balances to calculate source contributions. relies on correlations about the origin and a target rotation.

If fewer than 50 samples are available, the statistical significance of multivariate models is in doubt. A mass balance calculation can be used, this requires a source composition matrix assembled from specific source tests or literature values. If reentrained dust or fugitive emissions are suspected, then grab samples may be taken and analyzed as discussed previously. Since the variability of source compositions contribute to the overall uncertainty of the mass balance results, replicate analyses should be performed on samples of materials collected at several emission points within the same source so that average source compositions and their standard deviations can be obtained. Compositions for sources which cannot be sampled with Level II resources (e.g. smokestacks) must be obtained from literature such as is cited in Appendix B.

The mass balances are iterative, and several combinations of sources can provide equally valid fits to the receptor chemical concentration data (Watson, 1979). Judgement must be used to obtain a physically significant solution when using existing computer models.

The optical and scanning electron microscopy models combine the analysis and modeling together. Since neither the analysis nor the classification schemes in use are accepted by all researchers, analysis discrepancies described in Section 3 are often compounded by interpretation discrepancies, making the results semi-quantitative. Nonetheless, microscopy can provide conclusive source contribution results in certain situations. The cost of analysis per sample is also five to ten times the cost of the bulk chemical analysis used for input to the factor analysis, MLR and mass balance.

Microscopic analyses and models may be used in Level II to 1) confirm the conclusions drawn on a sub-set of samples by one of the other models and 2) to resolve anomalies found by these models. Note, however, that not all fine particles can be readily identified with microscopic analyses.

.4.4.2 Dispersion Modeling Analyses

e dispersion modeling analyses in a Level II study are more detailed and ally require more input data than the Level I analyses. Since it is ant to be able to determine source/receptor relationships on both a -term (e.g., daily) and long-term (e.g., annual) basis, techniques for ing both time periods are discussed in the following paragraphs. dures for modeling daily impacts are discussed first.

e primary objective of dispersion modeling is the reliable ification of source contributions. The screening dispersion modeling aches discussed in Level I provide a reasonably reliable and efficient to eliminate insignificant sources, but the simplifying assumptions yed can completely obscure the relative magnitude of the contributing e impacts. More reliable source contribution estimates can be obtained re detailed dispersion modeling analyses are performed.

n the following paragraphs, two different approaches are suggested for ore detailed short-term modeling analyses. The first approach can be to determine the relative magnitude of source impacts for 24-hour periods neral. The second can be used to do the same thing for specific 24-hour ds on which particulate matter sampling has already been conducted. The approach uses hypothetical meteorological data that are representative nditions that produce high concentrations of particulate matter. The d approach uses meteorological data actually measured on the specific when the particulate matter sampling was conducted. As a first step, approaches make use of the results from the Level I screening dispersion ing analyses to eliminate insignificant sources. Because of its superior ilities, the best model for both approaches is ISCST, although PTMTP, MPTER, and RAM could also be used. All of these models provide idual source contribution listings for each receptor.

In the first approach, the combined 24-hour impacts of multiple sources are obtained using a methodology patterned after the treatment of meteorological data in the PTDIS model. With PTDIS, 1-hour impacts (of a single source) are calculated using an array of combinations of wind speed and atmospheric stability. Likewise, the combined 24-hour impacts of multiple sources can be determined using a representative array of combinations of wind directions, wind speeds, and stabilities.

Each combination of wind direction, wind speed, and stability is input to the model to obtain a 1-hour average prediction. The impacts calculated for 1-hour periods are assumed to be representative of 24-hour periods. This simplifying assumption is reasonable because the monitoring site will receive the largest 24-hour impact from a given source if the wind direction is persistent. However, daily impacts will be overpredicted, primarily because wind direction variability is greater than is assumed here.

The large number of wind speed/stability combinations in PTDIS must be reduced to those combinations likely to persist for extended portions of a 24-hour period. Representative combinations are shown in Table 4-6. When some of these wind speed/stability combinations are used in the modeling it is necessary to consider the variability in atmospheric stability during 24-hour periods. Neutral ("D") stability conditions occur most often and can last 24-hours. Unstable ("A", "B" and "C") conditions occur only in the daytime and stable ("E" and "F") conditions occur only at night. Very unstable "A" conditions are likely to persist for only a few hours during the day.

Table 4-6 and the Level I screening modeling results may be used to select the wind speed/stability combinations for the more detailed modeling analyses. The PTDIS point source modeling results and the area, volume and line source modeling results from Level I are used to identify the 5 to 10

TABLE 4-6

COMBINATIONS OF WIND SPEED AND STABILITY THAT ARE LIKELY TO PERSIST FOR EXTENDED PORTIONS OF 24-HOUR PERIODS

	Wind Speed (m/s)	Pasquill Atmospheric Stability Classifications				
		Daytime Only			Nighttime Only	
		B	C	D	E	F
	2	✓	✓	✓	✓	✓
	4		✓	✓	✓	
tall stack sources	7			✓		
	10			✓		
						Rural areas only

highly dependent upon the source-receptor alignment relative to the input wind direction. A small difference (10°) in wind direction can produce an entirely different picture of the magnitude of the source impact at a given receptor.

There are two ways to ensure that the effects of wind direction are adequately considered. Either all compass wind directions (in 10° increments) can be modeled or only critical wind directions can be identified and modeled. The critical wind directions will be those associated with the sources that produce large impacts at the monitoring site. As mentioned previously, the Level I screening modeling results may be used to identify the 5 to 10 sources that have the largest impacts. In many cases, important sources will be found to be grouped together in one or two geographic sources that have the largest impacts at a monitoring site. The wind speed/stability combinations selected for further modeling are taken from among those that produced the highest impacts from those 5 to 10 sources. Table 4-6 also highlights a few factors that can be used to guide the selection of the most important wind speed/stability combinations.

Of all the meteorological parameters, modeled impacts at a given location are most sensitive to wind direction. The relative impact of each source is sectors. In that event, the wind directions can be input to the model in 10° increments from those sectors. Alternatively, the exact source/receptor alignment wind directions for selected sources can be input to the model.

Maximum impacts can be estimated using just a few wind direction/wind speed/stability combinations in the modeling. For the critical wind directions identified above, four combinations of wind speed and stability are suggested:

- low wind speed/unstable (B or C)
- low wind speed/neutral (D)
- low wind speed/stable (E or F)
- moderate or high wind speed/neutral (D)

Maximum 24-hour average impacts for each critical wind direction are then taken to be the largest of the hourly average impacts produced by either 1) the largest of the neutral stability impacts alone, or 2) by the largest of the neutral stability impacts averaged equally with the non-neutral stability impacts for a given wind speed. For example, for a given wind direction and wind speed, if the impact produced by B stability is larger than the impact produced by D stability, then the 24-hour average is assumed to be the average of the two hourly average values. Actual maximum 24-hour impacts will generally be a factor of 0.5 less than the values obtained above because of wind direction variability.

The second approach to the more detailed Level II dispersion modeling analysis depends on meteorological data recorded on specific days when particulate matter sampling has also been conducted. This approach is preferable if comparisons between measured and dispersion-modeled pollutant concentrations are anticipated. If the meteorological data are available, this approach has the advantage that the selection of meteorological input is simple. The meteorological data used in the model must adequately represent the actual meteorological conditions in the study area. As discussed earlier, modeled impacts are very sensitive to wind direction. For this reason alone, when modeling only involves a single sampling day and a single receptor, there is little likelihood of agreement between measured and modeled concentrations. The use of additional receptors in close proximity to the monitoring site will illustrate the sensitivity of predicted values to wind direction.

As mentioned earlier, it is often important to be able to determine source/receptor relationships on an annual average basis. A number of dispersion models are available for this purpose as shown in Table 4-4. The available models use either an annual stability wind rose or a full year of hour-by-hour meteorological data to calculate annual average source impacts. Procedures for using these models with a full year of data are contained in the respective model user's guides.

4.4.4.3 An Approach for Comparing Dispersion and Receptor Model Results

Comparisons between receptor and dispersion modeling results can provide important insights into source-receptor relationships. The two analysis approaches use different input information and incorporate different assumptions. The uncertainties associated with each approach can be substantial, but the similarities and differences between results from the two methods can often be used to identify erroneous or inadequate data and to achieve more reliable dispersion model predictions.

At the outset, the key to making comparisons between source (dispersion) and receptor modeling is to obtain source model results for the same monitoring periods when ambient measurements were collected. The sampling days selected for the analysis should represent a variety of dispersion conditions. The uncertainties associated with results from a single day are quite large; comparisons of results for a larger number of individual days (10 or 15 is recommended as a minimum) are more meaningful. The dispersion model used in these analyses must provide impact predictions for individual sources. The ISC models (ISCST and ISCLT) are best suited for this purpose because, in addition to the features described earlier, the ISC models will report impacts for selected groups of sources as well as for individual sources. The dispersion and receptor modeling results can then be compared on a source-by-source (or source group-by-source group) basis. Source groups are defined by the receptor modeling results, since receptor modeling does not distinguish among sources with similar emission compositions.

In the event that the receptor model results agree with the dispersion model results on a source-by-source basis, the receptor model analyses would constitute convincing evidence for the validity of the dispersion modeling analyses and vice-versa, since each will have been conducted independently. (As discussed previously, receptor model source contribution results should be established using two or more receptor models.) It is more likely that the source culpability information provided by the receptor model will differ considerably from that provided by the dispersion model, particularly for fugitive dust sources. In the latter case, validated receptor model results can be used to direct a re-examination of the dispersion model inputs to determine where inadequacies may exist.

The process of modifying the dispersion model or model inputs, based on comparisons between dispersion model predictions, observed ambient concentrations, and receptor modeling results, is primarily intended to identify and correct errors or shortcomings. The purpose of this exercise is to obtain more reliable, technically supportable dispersion model predictions, not to create the illusion of agreement between two problem-solving approaches. If reasonable results can be obtained through dispersion modeling, then a powerful analysis tool is available for estimating air quality at locations other than monitors and for assessing control strategy options.

The challenge is to accomplish this end in a systematic fashion, and to minimize the use of subjective, trial-and-error techniques. One effective device for controlling this process is the use of a "comparison protocol", which defines the stepwise analysis procedures to be followed once dispersion model and receptor model results are obtained. The protocol, prepared before modeling is performed, anticipates areas of possible disagreement between the two modeling approaches, identifies the model inputs and model features which could produce such disagreement, and outlines the decision criteria for revising the inputs or the model. Examples of the procedures such a protocol might contain are discussed below. The concept of a model comparison protocol is defined in considerable detail in the EPA document Interim Procedures for Evaluating Air Quality Models (U.S. EPA, 1981c). This document describes procedures for comparing the performance of two dispersion models and is not entirely applicable to the present topic.

There are a number of factors which cause dispersion model predictions to disagree with measured particulate matter concentrations. Some of these problems are source-specific, primarily affecting individual source-to-monitor impacts, while others are more likely to produce systematic or widespread bias in the model predictions. Examples of the former include:

- Erroneous emission rates caused by such items as the omission of unknown sources from the modeling or the use of inaccurate throughput information.
- The use of inappropriate emission rates, such as the use of total particulate matter emission rates which include particle sizes that settle out prior to impacting the monitoring site.
- Incorrect information concerning daily source operating parameters. For example, while a source may operate at 45 percent capacity on an annual basis, its actual mode of operation may be at 90 percent capacity for 50 percent of the days in a year.
- Neglect or incorrect consideration of downwash from tall stack sources.
- Neglect or incorrect consideration of resuspended particles.
- Building interference causing source-to-receptor (i.e., source-to-monitor) geometry to be incompatible with Gaussian dispersion assumptions.
- Local meteorology differing from that modeled. A typical problem is wind direction shift or channeling caused by buildings or topographic features.

Examples of factors that are not addressed by the dispersion model and that may cause systematic biases in model results include:

- Heat island effects which cause the actual near-source dispersion of elevated emissions to be greater than that modeled.
- Sea/land breeze effects.
- Effects caused by the fumigation of tall stack emissions.
- Effects caused by the development of thermal internal boundary layers (TIBL) over areas with varying surface heating characteristics.

There are also potential systematic and random biases in receptor models. Causes of such biases include:

- The selection of ambient sampler locations and filter samples for analysis such that the data studied are not spatially or temporally representative of the real air quality.
- Incomplete sampling schedules such that anomalous events are disproportionately represented in the data base. For example, samples may have been collected during periods of emission control equipment failure, or, in contrast, during periods when important sources were not operating. Conversely, a lack of such samples would also bias the data base.
- Incomplete or inaccurate information on source emission compositions, or the existence of sources with similar emission compositions such that the contribution of one source cannot be distinguished from that of another.
- Emission transformations where the amount or composition of emissions changes between the source and the receptor. Examples include particle deposition rates that differ among the chemical components, chemical reactions in the atmosphere, and the reentrainment of emissions that have already been deposited.
- Ambient sampling or filter analysis deficiencies where the data collected do not accurately reflect what is in the air. Examples include disparate collection efficiencies of the various filter media, artifact formation on filters, and analysis techniques that only see large particles, particles on certain parts of the filters or certain types of particles.
- Unrepresentative meteorological data. Examples include misoriented pollution roses and upper air trajectory analyses with directional and distance errors.

A three phase process is suggested to determine the need for making any changes in the dispersion model or input parameters. The first phase involves taking steps to eliminate obvious dispersion model input errors; the second involves modifying the dispersion model based on receptor model results for those sources whose input parameters are most certain; and the third involves the systematic comparison of predicted with measured concentrations to document model performance.

4.4.4.3.1 Phase 1. Refine Emissions Inventory. When large discrepancies are found between observed ambient concentrations and dispersion model predictions, emissions data are the first item to investigate. Receptor modeling results will indicate the contributions from different sources to observed concentrations. Comparison of source contributions predicted by receptor and dispersion model analyses will serve to focus attention on individual sources or source groups. Additional test data or more detailed engineering information can then provide a basis for inventory revisions.

Phase 1 can be accomplished through the following stepwise process:

- Identify "significant" sources or source groups from receptor model results. Sources which account for only a small fraction of observed ambient concentrations should not be investigated further.
- Assign a "level of confidence" to emission parameter estimates for each significant source or source group, based on engineering estimates and on receptor model results. Table 4-7 illustrates the confidence level information needed from this analysis.
- Obtain dispersion model results. Compare source contributions predicted by dispersion and receptor models. Identify any large, systematic discrepancies between source contributions from the two models.
- Re-examine the emissions data for sources with large discrepancies. Revise the inventory through additional source testing or improved engineering estimates, where confidence in existing data is low.

Recognizing that substantial uncertainty in particulate emission parameters and dispersion model predictions is unavoidable for most urban or industrialized regions, this Phase 1 effort is designed to focus attention on significant sources and on obvious errors. Analyses should be based on multi-day modeling results, rather than an individual day, since dispersion model predictions for short-term averaging periods can be very sensitive to small errors in plume transport direction.

TABLE 4-7

ASSESSMENT OF CONFIDENCE IN DISPERSION MODEL INPUT PARAMETERS

	Source Number/Type/Name							
	1	2	3	4	5	6	7	8
Source-Specific Errors								
Emission rate	3	1	etc.					
Particle size characterization	2	1						
Source locations/dimensions	3	2						
Source operation parameters	1	3						
Downwash	3	1						
Building interference	1							
Wind direction	2							
Other meteorology	3							
Other								

Key:

0 = Least confidence (in parameter or effect as modeled)
3 = Greatest confidence (in parameter or effect as modeled)

Confidence levels for emission parameters should be determined prior to dispersion modeling, to minimize the bias introduced by knowing in advance how well the dispersion model performs for any given source. Some receptor modeling techniques also provide quantitative estimates of the uncertainty associated with calculated source contributions. Model performance evaluation studies for dispersion models have shown that uncertainties of 20 to 30 percent are common for long-term average concentrations predicted at a given monitor location (Londergan, et al., 1983). Efforts to identify serious errors in the emission inventory should focus on sources with discrepancies of at least a factor of 2 between receptor and dispersion model predictions.

The pattern of discrepancies at different receptors may also aid in identifying potential inventory errors. For example, large overprediction by the dispersion model at a receptor very close to the source would suggest possible errors in source geometry; large overprediction at receptors far from a source would suggest an erroneous particle size distribution. Experience with dispersion models and emission inventories will play an important role in diagnosing potential inventory problems.

The protocol will serve as a check on the subjective process described above. The knowledge that a discrepancy can be "fixed" by increasing the emissions of a specific source is not sufficient grounds for revising the inventory. Technical justification will be required before changes are made. Through this process, however, efforts can be focused on the relatively few sources which are critical to dispersion model performance.

4.4.4.3.2. Phase 2. Further Dispersion Model Modifications. After the inventory revisions have been incorporated, revised dispersion model predictions will be obtained. The revised source contributions predicted by the dispersion model are again compared with receptor model results, to determine whether further modifications to the dispersion model or meteorological inputs are warranted. For this comparison, attention is focused on sources with the highest confidence rating for emission parameters and receptor modeling results. Any large, systematic discrepancies between dispersion and receptor model predictions for these sources would indicate shortcomings in either the receptor or the dispersion model.

The protocol will identify, in advance, the limitations inherent in the dispersion modeling approach. Such limitations may include meteorological inputs, assumptions concerning dispersion rates, particle deposition, effects of surface roughness or terrain, effects of land/water interface, etc. Remedial measures could include acquisition of additional meteorological data (if available), choice of different model options, or modification of dispersion algorithms to suit local conditions.

The pattern of model performance at different receptor locations and for different source types can provide useful information for diagnosing dispersion model shortcomings. Once again, however, emphasis should be placed upon large discrepancies between dispersion and receptor model results, recognizing the uncertainties inherent in both modeling approaches. Clusters of receptors, placed around each monitor, can be used to assess the sensitivity of dispersion model predictions to small changes in plume transport direction (and indirectly to indicate model sensitivity to one cause of prediction uncertainty).

Model modifications should be undertaken in an effort to improve performance by incorporating features which take into account local dispersion conditions and source characteristics. Problem-specific model modifications will often prove a cost-effective alternative to additional sampling and analysis.

4.4.4.3.3 Phase 3. Document Dispersion Model Performance. After revisions to the emissions inventory and/or the dispersion model have been implemented, it is important to document model performance using available monitoring data. Before the dispersion model is used to determine control requirements or to assess alternative strategies, the uncertainty associated with model predictions should be understood. For this purpose, observed and predicted ambient particulate matter concentrations should be compared, with primary emphasis on the concentration values associated with air quality standards (e.g., annual average and peak 24-hour concentrations). The comparisons should not be restricted to those days selected for receptor model analysis, but should include at least one year of ambient monitoring data. The meteorological data used should correspond to the particulate matter sampling schedule.

Detailed recommendations concerning model performance evaluation are contained in the reports Judging Model Performance, from the 1980 American Meteorological Society (AMS) Workshop (Fox, 1981), and Interim Procedures for Evaluating Air Quality Models (U.S. EPA, 1981c). In the present context, a limited analysis of model performance is envisioned, rather than the comprehensive statistical evaluation described in these reports, but the basic analysis approach is quite similar.

Results from the performance evaluation will provide a basis for deciding whether to rely upon the dispersion model to formulate control strategies, or whether to use monitoring data and receptor modeling results. If the dispersion model is demonstrably reliable at the monitoring sites then model predictions can be made for the entire study area and control strategies should be developed based on the model results. If the dispersion model is not proven reliable, and measured concentrations show nonattainment, then control strategies would be developed based on the measured data and receptor modeling results. However, in this case, the issue of the air quality at non-monitored locations must be addressed. If the monitoring sites are not representative of the entire study area, based on dispersion model predictions, then additional monitors may be needed at locations of high predicted impact so that additional receptor modeling analyses can be used to determine the source impacts at such sites.

4.4.5 Resources

Resources required for Level II analyses are significantly higher than those required for Level I. At least a mini-computer is required to run programs, not all of which are in the public domain at this time. Data bases are large and require sufficient storage. The analyses described here should not require substantial additional monitoring, but it will usually be necessary to perform a variety of laboratory analyses on existing samples. Analysis costs will range from $25,000 to $100,000. Four months to one man-year of effort will be required.

4.5 Level III: New Sampling, Analysis, and Model Development

The frequent need to solve problems associated with atmospheric pollutants, other than those materials collected routinely by monitoring networks, requires the development of sampling and analysis strategies specifically directed to the individual problem. In many cases, these problems can be explored using receptor models or dispersion models and can use readily available sampling and analysis methodologies. However, sometimes it may be necessary to incorporate vastly different approaches into the study design. A few examples would be programs to define the sources of 1) sulfate,

2) organic particulate matter, and 3) the mass of material in particular size fractions. For each of the above, a similar general approach can be used in the design of the experiment; however, the details for each case require considerable discussion.

The following is structured to establish general criteria for the development of Level III studies.

4.5.1 Source Data

As has been described in other sections of this volume, and other volumes of this series, a major concern is the availability and subsequent cataloging of source emissions data for both receptor and dispersion models. In Level I and II, the methodology for acquiring useful information from existing source emissions data bases was described. However, these will probably be inadequate to address many specific air pollution problems because all the sources, or at least the major sources, in a particular study area may have only been tested for a limited number of parameters. Furthermore, some data bases were not designed to mimic the emission patterns that would more closely represent the physical and chemical fractionations and transformations that occur in the environment and are observed in receptor samples (for example, sulfate and organic species). Such a deficiency is important when using a receptor model to allocate the percent of mass associated with a source or when trying to validate the model with some contribution estimates from appropriately parameterized dispersion models.

The first stage of Level III is to draw upon the previously acquired data in Levels I and II and outline a strategy based upon the strengths and weaknesses of available emissions inventories. At present, these data could be augmented by conducting actual source tests similar to those normally used the federal New Source Performance Standards (NSPS) or National Emission andards for Hazardous Air Pollutants (NESHAP) programs, but adding trace ement and other chemical analyses would be required in the development of arce compositions for input to receptor models. In most cases, the rticulate matter size fractionation would not have been attempted, and the sults would be useful only if the chemistry of the emissions does not vary preciably between size fractions.

In place of the above, the critical question of compatibility of the urce compositions with those perceived at the receptor could be addressed ing dilution sampling or platform sampling downwind of plumes. These chniques could also estimate the mass emission rates under a variety of erating conditions. A selection criteria for the sources to be tested ould be established based upon 1) the adequacy of cataloged profiles (with ncern for regional differences in sources), 2) the emission rates of urces, 3) the proximity of the source to the receptor site, and 4) the tential hazard associated with the source. Additional source testing iteria are discussed in Section 2.2 of Volume II of this series (U.S. EPA, 81b).

Dilution source testing has been identified as a method to help increase e possibility of having the source composition more closely reflect that mpled at a receptor. It involves cooling of the sampled effluent to a mperature which is nearly equivalent to that found in the ambient vironment to simulate the conditions under which condensation, growth and her reactions of the emitted species occur. A further distinct advantage is e possibility for sampling the diluted effluent with techniques equivalent those used at the receptor. In the case of particulate matter, the net sult could be the development of source composition catalogs which would be size classified and/or be able to capture more volatile species. As mentioned in previous volumes of this series, a present drawback is that this sampling is still in the development stage. Therefore, a standardized sampling methodology is not available as of this writing.

Another approach to the collection of emissions at conditions which are more nearly equivalent to those anticipated at a receptor would be platform plume sampling. In the past, this methodology has been used in dynamic experiments (Lagrangian coordinate system) where the production and transport of ozone and secondary particulate species were studied in both urban and power plant plumes. However, plume sampling can be accomplished in an Eulerian experiment (fixed coordinates) by measuring the plume at a fixed point with a suspended platform (skyhook, etc.) near the receptor. Obviously, because of the expense, major sources along the prevailing wind direction should be of prime consideration and the sampling platform, fixed or otherwise, must have collection devices which are nearly equivalent to those used at the receptor. Preliminary or informational studies on the anticipated emissions should be completed so that the plume sampling is well focused. As stated previously, the sampling should be size selective (one or two stage) for particulate matter in order to accommodate future regulatory requirements and to differentiate between the fine and coarse fraction compositions.

In some types of studies, ground based plume studies may also be warranted. This technique will be quite useful for receptor sites located near major automobile and truck traffic arteries, farmlands spraying pesticides, fugitive dust emissions, and field burning activities. Properly outfitted vans or temporary trailer monitoring stations can be used to house equipment.

The source characterization used in Level III studies will be directed toward achieving the most representative compositions of the sources that can affect a receptor. It will combine information available from Level I and Level II activities with new source tests. These latter tests will be designed to be conducted at conditions more closely associated with the ambient environment. To reduce costs, each should be conducted at times when ambient samples are collected at the receptor and the receptor is downwind of the source.

4.5.2 Meteorological Data

The Level I and II approaches to source or receptor modeling involve the accumulation of readily available meteorological data from NWS, State and local government or privately operated stations. In addition, synoptic or mesoscale meteorological data are processed via computer programs to give either upper air or surface wind trajectories. In many cases, this is all the resolution that may be required, since these data are available near most major urban centers. For multivariate receptor modeling techniques the same resolution is sufficient such that with large numbers of samples (200-400), it will be possible to categorize the apportionment of a given species according to wind direction. The trajectory analyses will also prove useful in attempting to determine the contributions of chemical or other species from local versus regional sources.

In a Level III study it is possible that the meteorological detail will need to be more extensive. This would be especially important in situations where the influence of complex terrain, sea breezes or valley channeling will distort the local wind and atmospheric conditions to such an extent that the Level I and II meteorological data will be unreliable and comparisons of dispersion and receptor models will be difficult. In addition, there will be situations where the available meteorological stations are too distant or, for various reasons, are not sufficiently representative of the study site. It is important to note that although the mass balance for particulate matter requires as little as one sample to estimate the percent contribution from individual sources, the support data requirements are significant. Depending upon the location of the site, more samples will have to be taken for various meteorological conditions to assess the frequency and magnitude of sources influencing an area.

The Level III approach to meteorological data acquisition will require location of a meteorological station either at or in close proximity to the sampling location. For example, in the New Jersey ATEOS study (Lioy and Daisey, 1983) the monitoring sites were within 10 miles of an airport NWS site which eliminated the necessity for a local meteorological station. It should provide, at a minimum, the types of meteorological data available on the local meteorological data summary provided by the NWS from airport sites located in the United States. However it would be advantageous to also have data on the mixing height and the wind profiles at altitudes above the surface. While there are various means of obtaining such data, it would be preferable to install an acoustic sounder at a suitable location. This device is versatile and will provide computerized output of meteorological information on a real time basis (continuous) throughout the day. Indirect measurements made by doppler type acoustic sounders include the wind speed, wind direction, vertical motion, standard deviation of vertical motion, horizontal components of turbulence, and echo strength (proportional to the temperature structure of the atmosphere). In addition, with the use of appropriate algorithms, the echo strength can be converted to mixing height.

These devices can be operated for long durations, as long as there is proper maintenance and periodic review of the data. The mixing height and wind parameter data from the acoustic sounder will in fact provide a useful way to estimate the burden of atmospheric pollutants of local origin versus the amount associated with the regional background pollutant concentrations (Gaynor, 1977).

4.5.3 Ambient Data

4.5.3.1 Size Selective Sampling for Particulate Matter

As stated previously (Levels I and II) the majority of available data for particulate matter has involved the total mass collected on a hi-vol or dichotomous sampler. The hi-vol has a nominal 50 percent cut size of 30-40 µm which indicates that large quantities of coarse materials (perhaps from fugitive dust sources) will be collected.

Over the period extending from 1973-1983, an increasing number of studies has been conducted by various organizations in which size selective sampling of the particulate mass has been completed and composition data reported. In many cases, a dichotomous sampler with a 2.5 µm and 15 µm 50 percent cut size was used for fine (respirable) and coarse particles. This appeared to help differentiate sources in the specific cases used for source apportionment studies (Dzubay, 1980; Kneip, et al., 1983; and Dzubay, et al., 1983.) However, size selective inlet samples (15 µm cut size), multi-stage impactors, two-stage cyclone filter samplers and various other techniques have been used to collect particulate mass samples.

These samples are collected on filter media which are then processed by a variety of techniques for elements, inorganic compounds and organic compounds. An up-to-date review of filter media and the concerns for sampling and analysis has been published by Lippman (1983).

Unfortunately, an all purpose sampler has not been developed; however, several observations can be made. If the intent of the studies to be conducted is on sources of sulfate, total carbon or size fractions of the particulate mass, the dichotomous sampler would be the common sampling device used for air pollution measurements. However, if the concern is for species which need large quantities of samples in order to be above the detection limit, such as polycyclic aromatic hydrocarbons or other organic species, a different sampler with the appropriate size selective inlet would be required for the study.

4.5.3.2 Time Resolution

This aspect of sampling is always difficult to judge precisely. The purist would want to have a continuous record or at least frequent samples in a given day. The pragmatist must make a cost effective compromise. What is actually necessary is good planning, based upon the type of the pollution problem suspected as well as the modeling techniques to be used for the source apportionment studies. Traditionally, 24-hour sampling periods have been found to be adequate for measuring the particulate matter levels and long-term variations and trends in an area.

In the case of 24-hour samples, a large number of samples (≥ 50) are required to conduct multivariate analyses. In addition, these would have to be either spaced over the seasons of the year or conducted in the same season over a number of years. For mass balance techniques, much fewer samples are required because the mass balance analysis can be performed on a single sample. The number of samples required is determined by the extent of the need to assess the problem on a 24-hour or annual basis.

Alternatively, to focus on one particular source or to examine diurnal ifferences, a series of shorter duration samples could be taken (from one to ix hours in duration). Stricter requirements will then be necessary for the eteorological support data, and appreciation of seasonal differences must be oted in the sampling strategy. In addition, these short-term samples must ontain enough material (mass of particulate matter) to make is possible to erform gravimetric and chemical analyses.

Finally, in all receptor modeling studies that have used catalogued source rofiles, the adequacy of those profiles for representing emission conditions uring the sampling period is always a serious consideration. Therefore, any ew source test should be done as close to the time of sampling as possible.

4.5.3.3 Composition Determination

The previous volumes in this series and other articles, including the esults of the Quail Roost Workshops I and II have discussed, for possible use n receptor models, a number of species and their limits of detectability. In olume II of this series, much time was spent on species which should be etermined for the mass balance technique. However, the use of other pproaches including multivariate modeling and electromicroscopic identiication would have different requirements. To compound this problem, the evel III approach may deal with some very unusual problems. Therefore, the election of the correct list of species for analysis may require substantial nformation gathering studies prior to the development of an analytical rotocol.

4.5.3.4 Prioritization of Chemical Analysis

After selection of the variable (dependent) to be apportioned, a variety of chemical analyses will be completed on the collected samples. The optimum situation would be analysis for all species associated with the sources that potentially will affect the site. However, some caution must be exercised since this approach may, in fact, ignore a source that was not identified in Level I or Level II studies.

Prioritization of the analyses to be completed is a necessity for cost controls, and those species selected must, in many ways, be tied to the objectives of the Level III study.

The case of particulate mass sampling (total or size fractions) is a good example from which to develop some general analytical guidelines.

- Particulate Mass: Since this is the dependent variable in receptor models, and the objective of source/dispersion models it must be measured. In traditional studies, it was TSP; however, this measurement could be of a particular size selected fraction. (In other cases, the material to be apportioned could be SO_4^{-2}, carbon, organic compounds, etc.).

- Trace Elements: A majority of the information that has been obtained from previous receptor modeling has come from trace element source signatures. These will be of great necessity in any Level III study. In fact, these data will be required for both source and ambient samples since size selected studies will probably become more frequent in the future and relatively few particle size fractionated source test results are available.

  Methods for elemental analysis described in previous volumes indicate that the multi-element approach (as opposed to unique tracers) seems to be the most effective. For each study, the method of choice must be critically evaluated to prevent the exclusion of a major element from the analysis. Morphological studies may also be necessary to further assist in source identification (see Volume IV, U.S. EPA, 1983b, for details).

- Inorganic Ions: In most instances, except those where one source dominates the collected particulate mass, various anions (and their cations) will comprise significant portions of the particulate mass. Therefore, the immediate thought is to incorporate them into a receptor modeling study. Before this is done, however, the partitioning between primary emissions and secondary products, and the fractionation according to particle size must be considered. Differentiation will assist in local versus distant source allocations. To accomplish the task, a Level III study may require a large amount of ambient samples and meteorological data for the development of multivariate models and before such information can be used in a mass balance study. Without partitioning of the local and regional contributions, the primary value of the ion data will be for composition rather than apportionment of sources. In the case of inorganic ions such as sulfate, the combined use of dispersion and receptor models will be advantageous in helping differentiate local contributions.

- Organic Matter: There are a number of different levels from which to approach the use of total organic matter or individual organic compounds in a receptor model.

  - Extractable Organic Matter (EOM): Depending upon the fraction of EOM examined, the extractable mass data can give information on primary organic material and potentially on secondary organic material. These types of data are useful in further defining the sources of the material affecting a receptor. However, these data may in fact be more effectively used as the dependent variable in an organic particulate matter source apportionment model.

  - Organic Carbon/Elemental Carbon/^{14}C: These data are available from previously described analytical techniques, and can be used for assisting in the apportionment of particulate mass in the atmospheric samples. Emission tests and ambient sampling can be completed for carbonaceous material. Therefore, if these data can be obtained in the same samples as the trace elements, the ability to differentiate sources may be extended. A particularly promising tracer is that of $^{14}C/^{12}C$, which may be useful in identifying the contribution of "contemporary" carbon sources, such as woodburning in fireplaces and stoves.

    As in the case of EOM, these materials can also be used as the dependent variable in a receptor model if the appropriate emission inventories are available for use in a mass balance model. However, a thorough catalog of sources would not be a requirement for use in a multivariate model apportionment study.

  - Polycyclic Aromatic Hydrocarbons (PAH): Because PAHs found in airborne particulate matter are the most carcinogenic component in animal bioassays, they may present major concern to the public health. However, for apportionment studies, they can be used in three ways: 1) specific PAHs can be used as tracer variables for combustion processes; 2) as the dependent variable in a receptor model or 3) as an emissions term in a dispersion model. Depending upon the type of data (source and ambient) either mass balance, factor analysis or multivariate target transformation or multiple regression techniques can be used to analyze these data in receptor models.

One caution which must be mentioned on this topic - the partitioning of each PAH between the gaseous and particulate phase must be considered before it is used in a receptor model or dispersion model. In some cases, such as Benzo-a-pyrene (BaP), this may be insignificant. However, for other compounds a temperature dependence may be apparent and will affect the validity of any apportionment conducted.

- Other Materials: Most of these may be available from routine monitoring data, and can be useful either as the dependent variable or as further qualitative information to define sources. The primary species include: CO, SO_2, NO_x, O_3 and HC. However, in the future, volatile organic compounds will probably gain in importance from the point of view of toxic substances, photochemical smog precursors, and as source signatures.

4.5.4 Procedures (Level III)

It is assumed that Level I and Level II and what has been discussed previously in Level III is in place, or is available for use. In designing a source/dispersion modeling study, one would select the monitoring network which most closely reflects the majority of source-meteorological factors (such as prevailing winds, sea breezes, etc.) that may be encountered in a region. Thus, the maximum number of sites would be dependent on a coverage factor for the area source, frequency of meteorological conditions and strength of source.

Unfortunately, the case is not as simple for a receptor site which would be an impact site for individual sources that are examined by the dispersion model. Such a site can be influenced by many different sources depending upon the season or daily meteorological conditions. A major concern would be coverage by secondary sites surrounding the primary receptor site. Sometimes, if a large urban area is to be studied, more than one receptor site could be chosen since each may be representative of different activities of the area. For instance, the sites could be distributed in downtown commercial, residential, or industrial areas. Obviously, in each case, a different aspect of an air pollution problem will be examined and the final selection of the number of sites would be dependent upon the overall goals of the investigation. For instance, the sites selected for examining TSP or some size fraction in an urban nonattainment area might not necessarily be equivalent to a site where there is a potential impact of hazardous materials in a residential section. For a TSP or PM_{10} study, two or three sites at different locations may be warranted. In the latter case, one or two sites may be used as the receptors in the same neighborhood.

Once the primary site or sites are selected, of utmost importance is the selection of a rural site located on level terrain away from significant local sources and meteorological perturbations. These sites must provide coverage for the dominant wind directions; however, in many cases, at least two "upwind" sites, i.e., along the dominant wind paths, should be required although anywhere from 1 to 4 sites are conceivable. Under no circumstances should the study be done without at least one background site.

A primary consideration at the rural sites is the travel time and technician time needed to obtain the samples used for determining regional or background levels of pollutants. Obviously, the major species should be measured as should the major tracers. Beyond that, it depends upon the availability of resources. The optimum situation would include completion of the same set of analyses on the background and urban samples (receptor).

The sampling duration and sampling frequency will have been determined prior to site selection; however, there should be some flexibility in the design. It may be necessary to adjust the sampling schedule if a major event occurs, unexpected results begin to appear, or unanticipated problems arise. Crucial in all these studies is the development of an adequate sampling and analysis quality assurance program. Without this type of control on the study, the results may be less than adequate for use in model development. In essence, error terms must be minimized. EPA guidance on the preparation of quality assurance plans is contained in a document entitled Interim Guidelines and Specifications for Preparing Quality Assurance Project Plans, (U.S. EPA, 1980c).

The final aspect of this study design is the model development and a number of a priori issues must be considered. At a minimum for dispersion model validations, the cases selected require short duration samples and the periods chosen should adequately reflect the emissions inventory or operating parameters that could be in effect at that time. Thus, for example, the analytical protocols could involve the following steps:

- Dispersion models are to be run using the source emission inventories developed in Level III.
    - Selection of meteorological parameters corresponding to those observed during the sampling study.
    - Selection of emission conditions which would closely approximate the emission strengths that occurred during the sampling period.
- Complete a mass balance or microscopic analysis on a particular sampling day (or on days selected to represent an annual average).
    - Select a sampling day during which the source is more nearly upwind of the receptor site.
    - Complete mass balance or microscopic analysis on that day and estimate mass contributions.
- Compare the dispersion model source contributions with those of the receptor model. Those contributions estimated by each model which do not differ by more than the sum of their uncertainties are consistent. This consistency provides a good basis for justifying a control strategy applied to these sources. The dispersion model may be re-run for individual sources within one of these source categories to specify which one might result in the greatest pollution reduction per dollar spent.

- If source and receptor model results differ by more than the sum of their uncertainties, the data on which both operate need to be refined. The nature of this refinement is often indicated by the model results.
    - If the receptor model identifies a source contribution which wasn't included in the emission inventory for the source model, an inventory for that source must be carried out. Wood burning (Core, et al., 1982) was discovered as a major source by this procedure.
    - If the receptor model finds a "downwind" source to be a major contributor, meteorological inputs to the source model should be examined and improved.
    - If all source type contributions calculated from the source model are high or low with respect to the receptor model, the source model should be re-run with revised or corrected stability and mixing height data.
    - If model calculations differ by a factor or two or more, the emission factors and positions of the gridded emissions inventory for the source model should be double checked. Alternatively, additional source characterization tests for the receptor model may need to be made. By confining these activities to major contributors with major discrepancies, the work can be focused with great savings of effort over verifying all source emission rates and compositions.
- When the data have been refined, both models should be re-run and the two preceding bulleted steps should be repeated.
- If comparisons are still inadequate for decision-making purposes, and if the cost of a wrong decision merits it, artificial tracers may be introduced into the questionable emissions, simultaneous measurements may be made at both the source and receptors, and source and receptor models may be re-run to identify where the discrepancy lies. The basic assumptions and structure of the models may have to be modified as a result.

Concurrently, the mass balance results should be intercompared with studies that use any one of a number of microscopic techniques. Comparisons with other mathematical techniques such as factor analysis or multiple regression, or combinations of techniques such as target transformation factor analysis, or factor analysis with multiple regression, may be useful. Conversely, if microscopic methods are the primary receptor models used, they should be intercompared with mathematical methods. In these cases, the sources' contributions to a percentage of the mass will be determined. The results must be compared for consistency and errors.

4.5.5 Resources

Resource requirements for level III are large. A mini- or main frame computer will probably be needed to store data files and to operate comprehensive programs. Since new sampling programs will be conducted, the requirements for monitoring equipment, personnel and laboratory analyses will be sizeable. Manpower requirements may encompass man-years and study durations can extend to a year or more. Costs will range from $100,000 to over $1,000,000.

4.6 Summary of the Three Level Approach

Studies conducted to determine contributions to measured particulate matter concentrations can require different levels of effort. The level of effort required in each case will depend on the nature and extent of the problem and on the amount of information already available. This volume organizes the analyses used to solve source apportionment problems into a three level format. Table 4-8 summarizes the various aspects of the three levels of study. The three level format is flexible and the information in Table 4-8 should not be rigidly confined to each study level. In real world applications, there may be intermixing of components of the three levels due to data and resource availability.

Two items are applicable to all three study levels. First, an analysis of background concentrations is an essential preliminary step to the other analyses in each level, and second, two or more source apportionment methods should be employed, if possible, at each level in order to provide greater confidence in the study results.

TABLE 4-8
SUMMARY OF THE THREE LEVEL APPROACH

ACTIVITY	LEVEL I	LEVEL II	LEVEL III
Brief Description	• Uses existing data, requires no new monitoring • Accomplished with simple, straightforward analyses • Generally uses qualitative receptor models, screening dispersion models • Identifies likely contributors, eliminates likely non-contributors, focuses subsequent efforts • May provide conclusive contributions for some situations	• Entails new analyses of existing samples, limited new monitoring • Performed with advanced use of standard techniques • Generally uses more quantitative receptor models and refined dispersion models • Usually conclusively identifies and quantifies source contributions	• Involves new sampling programs • Sophisticated analyses developed and used • Addresses site-specific problems such as sea breezes, complex terrain, multi-source areas, transport • Dispersion and receptor modeling analyses geared to quantitative identification of source contributions
Source Data	• Emission rates and source configuration parameters[1] • Source location coordinates or maps[2,3] • Particle size and composition of emissions • Temporal variability of emissions[3,4] • Libraries of emission compositions by source type[4] • Emissions grouped by source type, tracer elements[3,4]	• Confirm emission rates from material throughputs, control efficiencies[1] • Documentation of source configuration parameters[1] • Libraries of emission compositions by source type [2,3] • Microinventories and sampling day inventories[3,4] • Collect emission composition samples for selected sources - grab or stack tests[3,4]	• New source testing for emission rates using standard techniques (NSPS, NESHAPS)[1] • New source testing for size fractions, chemical compositions[2] • Dilution effluent, platform plume, ground-based plume sampling[3,4] • Emissions tracer testing[3,4]
Meteorological Data	• Hypothetical hourly surface wind speeds, temperatures, atmospheric stabilities, mixing heights[1] • Resultant surface wind speeds and directions[2] • Annual or seasonal precipitation totals[2] • Daily average wind speeds, temperatures, mixing heights[4] • Daily weather maps, upper air wind summaries[4]	• Actual (or hypothetical) hourly surface wind directions and speeds, temperatures, stabilities, mixing heights from representative locations for selected days[1] • Daily surface resultant winds, temperatures, mixing heights, precipitation, weather maps, upper air winds[4] • Computerized hourly surface and upper air parameters[3] • Computerized daily surface and upper air parameters[4]	• On-site monitoring for horizontal surface winds[1,2] • On-site monitoring for temperature, vertical wind profiles, mixing heights, vertical air motion, turbulence[3,4]

1. Needed for dispersion models
2. Needed for receptor models
3. Helpful for dispersion models
4. Helpful for receptor models

TABLE 4-8 (Continued)
SUMMARY OF THE THREE LEVEL APPROACH

ACTIVITY	LEVEL I	LEVEL II	LEVEL III
Ambient Data	• Particulate matter concentrations from hi-vols, size-selective hi-vols or dichotomous samplers[2] • Particle constituent concentrations from such samplers, including particle size, chemical compositions[4] • Monitoring site survey results[4] • Previously collected filter samples[4]	• Particulate matter concentrations from size-selective hi-vols or dichotomous samplers[2] • Particle constituent concentrations from such samplers (chemical compositions)[2] • Previously collected filter samples[2] • Limited new sampling[4]	• New sampling for total mass, size-segregated constituents[2] • Specific new sampling for sulfate, carbon[2] • Specialized new sampling for organic species[4] • New sampling for hourly, diurnal, etc. time periods[4] • New sampling for specific mass loadings required by certain laboratory analyses[4]
Resources	• Minimal computational capabilities required (desk top calculator) • Study time frame short (weeks to months) • Manpower needs minimal (one to three man months) Little or no monitoring or laboratory analyses needed • Costs range from $5,000 to $25,000	• Mini- or main frame computer may be necessary • Moderate study periods required (months to year) • Manpower requirements modest (man months to year) Minimal monitoring, moderate laboratory analyses • Costs range from $25,000 to $100,000 •	• Mini- or main frame computer probably necessary • Study durations lengthy (at least one year • Manpower requirements considerable (man-years) • Extensive monitoring and laboratory capabilities required • Costs range from $100,000 to $1,000,000

1. Needed for dispersion models
2. Needed for receptor models
3. Helpful for dispersion models
4. Helpful for receptor models

5.0 CASE STUDIES OF COMPOSITE SOURCE APPORTIONMENT METHODS

There are a significant number of examples where composite source apportionment methods have been used effectively to answer questions on the degree to which various source categories cause a nonattainment situation or other air quality situation of interest. These studies cover the full spectrum of complexity from Level I to Level III. Since the dividing lines between the three levels of complexity are not clear cut, it follows that many of the case studies may contain analyses that might logically be part of more than one complexity level.

The following case studies exemplify the three levels of complexity of composite source apportionment methods.

5.1 Use of Microscopy and Filter Analysis (Level I)

Draftz, et al., (1980) of the Illinois Institute of Technology Research Institute (IITRI) have developed a protocol using microscopic identification of particles collected on hi-vol filters supplemented by chemical analyses of the filter deposits to apportion the collected particles to various source categories.

Polarized light microscopy is the principal tool used to identify particle sources based upon the previous microscopic analysis of particle samples collected from various sources. X-ray diffraction may also be used to provide positive identification of mineral species and scanning electron microscopy may be used for identification of extremely small particles.

Low temperature ashing is used to determine the organic content of the collected particles. Ion chromatography is used to determine the anions and cations present, and depending on the nature of the study, elemental analysis of samples may be carried out using x-ray fluorescence.

Data are presented in terms of percent contribution of source categories such as combustion, specific metallurgical operations, road traffic, and biological aerosols.

5.2 Linn County, Iowa Non-Traditional Fugitive Dust Study (Level I)

A recently conducted study by Brookman (U.S. EPA, 1983d) investigated the primary non-traditional sources affecting the air quality in and around Cedar Rapids, Iowa (Linn County). The approach used for this study was, essentially, the Level I protocol involving many of the analysis discussed in Section 2.3.7.

The data base used for this study included existing source, meteorological and ambient data. The source data were in the form of existing microinventories around the five county monitoring stations and one rural background station, a point source inventory performed by the local agency, and a "first-cut" area source inventory (part of this study was to update this inventory and then use the results for the nonattainment study). The source data were supplemented with topographic maps, aerial photographs, and an industrial fugitive source inventory (performed as part of the project). The meteorological data were obtained from the Cedar Rapids Airport in the standard form of LCD's (Local Climatological Data Summaries). The ambient data were obtained from the State authorities and consisted of seven years (1976 - 1982) of hi-vol data collected at the one background and five county stations.

The first step of the protocol was to visit the monitoring sites to get a "feel" for local contributing sources, topographic anomalies, siting characteristics, etc. The second step was to evaluate the meteorological data. This included determining wind persistence for each of the sampling days during the seven year period and noting precipitation and snow cover on and preceding the sampling days. The third step was to determine the background level for each year of the study period. This was done by using the rural station hi-vol data. This level was found to be highly variable from year to year, in direct correlation with the amount of precipitation for that year (in fact, a linear relationship was shown to exist).

The next step in the protocol was to perform a trend analysis (see Section 2.3.7) and remove the background influence (thus effectively removing the meteorological influence). The resulting trend plots for the five stations showed definite anomalies at certain stations during certain years. Further analyses were performed to try and discover the reasons for these anomalies. First, the modeled point source influences were removed from the yearly averages (the State has performed ISC modeling and information was available on the relative monitor impact for each year). Second, pollution roses were developed based on days with persistence greater than 0.71 (see Section 2.3.7). A pollution rose was also developed for the background station and its influence was removed from the county station pollution roses.

Using the results of these basic analyses in conjunction with the topographic maps, aerial photographs, site visits, discussions with County officials, etc., probable causes for the nonattainment status of several monitoring stations were uncovered. The principal findings of the study showed that highway construction was the principal cause of TSP violations at several stations throughout the years, industrial fugitive sources contributed several micrograms per cubic meter to a few stations, and vehicle traffic on paved and unpaved roads contributed heavily to most of the stations. The results also showed that there was a general downward trend in the TSP levels throughout the county throughout the years as a result of control programs (street cleaning, paving) and the economic recession (several large industries had cut back their operations significantly).

The results of this study, which was conducted entirely using existing data, were very helpful to the local authorities in planning future control strategies (particularly in regard to construction projects). Example results for one of the five monitoring sites are shown in Table 5-1. While the Level I approach could not determine exact levels of source contributions or distinguish between several fugitive sources in the same area that were probably affecting a monitoring station, it did provide the authorities with all of the information they desired. The next logical step for further source contribution quantification would have to entail microscopic analyses of filters and/or directional sampling.

TABLE 5-1

ESTIMATED SOURCE IMPACTS AT ONE LINN COUNTY, IOWA
MONITORING LOCATION (EQUIVALENT GEOMETRIC MEANS $\mu g/m^3$)

Source Type	Year 1976	1977	1978	1979	1980	1981	1982
Background	47.0	38.6	37.9	35.8	40.7	36.5	26.0
Traditional:							
Stack	8.8	8.8	8.8	8.8	8.8	8.8	8.8
Fuel Combustion	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Solid Waste Disposal	2.1	2.1	2.0	1.8	1.7	1.5	1.4
Auto Exhaust	2.7	2.7	2.7	2.7	2.8	2.8	2.8
Annual Recorded Mean	98.8	109.3	90.6	95.0	106.5	80.0	60.9
Non-Traditional Impact	37.2	56.1	38.2	44.9	51.5	29.4	20.9

5.3 Allegheny County Particulate Study (Levels I and II)

A study was carried out in Allegheny County (Yocom, et al., 1979, and Brookman and Yocom, 1980) to investigate the particulate matter nonattainment problem in the county and to determine the types of sources primarily responsible for the nonattainment situation. Of particular interest were the relative contributions of the following types of sources:

- Traditional - Industrial point and process fugitive sources.
- Non-Traditional - In-plant open sources such as roads and material piles and non-industrial sources such as public roads and playgrounds.
- Background - Natural sources and sources outside the county.

This study was an example of a composite source apportionment method applied principally to available TSP data collected by the County Bureau of Air Pollution Control. Most of the methods described in Section 2.3.7 (Preliminary or Qualitative Receptor Models) were applied to this data base. Dispersion modeling using a version of PAL together with a detailed inventory of traditional and non-traditional sources at the large, integrated steel mills was used to predict specific contributions of these sources on selected sampling sites.

Background levels of particulate matter were determined by the "composite particulate rose" method described in Section 2.3.7 and applied equally to all sampling sites in the county.

The assumption was made that the industrial component of measured particulate matter at stations near the steel mills was made up entirely of steel mill contributions. These stations constituted most of the nonattainment stations. A variety of techniques (e.g., pollution roses, wet/dry day analysis, microinventories, etc.) was used to infer the relative contribution of traditional and non-traditional sources for the remaining sampling stations in the county.

Special short-term sampling runs using Millipore filters were carried out at several of the sampling sites under predetermined meteorological conditions. These samples were subjected to automated scanning electron microscopic and energy dispersive x-ray analysis (SEM/EDAX) to determine the chemistry of the selected particles in relation to particle size. By making certain assumptions on the contributions of traditional and non-traditional sources to specific particle chemistries it was possible to reconcile the dispersion modeling-plus-background source apportionment results with those of the particle identification studies.

Using estimated predictions of future reductions in emissions from traditional and non-traditional industrial sources, the number of nonattaining stations decreased and strategies could be developed for bringing the remaining nonattaining stations into an attainment status by application of controls on various categories of non-traditional sources.

The actual contracted cost for this study was about $60,000 in 1978 dollars. However it should be pointed out that the contractor served as a consultant and management contractor and was asked to utilize much available data and systems. One important feature was that 5 years of TSP and meteorological data were already up on a large computer and were readily accessible for a variety of manipulations. Furthermore, the dispersion modeling and steel mill inventory were carried out by another contractor under the sponsorship of a steel company consortium, and the special sampling and SEM/EDAX work was funded directly by the county with yet another contractor group. Thus the total costs for the project were estimated to be in the range of $300-500,000.

5.4 Portland Aerosol Characterization Study (Level III)

The Portland Aerosol Characterization Study (PACS, Cooper, et al., 1979; Watson, 1979; Core, et al., 1982) is a classic example of a Level III study.

Its purpose was to quantify the major contributions to TSP concentrations which were in violation of the NAAQS. It involved the following elements:

- Creation and use of a site specific air quality dispersion model (Fabrick and Sklarew, 1975).
- Multiple site meteorological monitoring to create a complex wind field.
- A site specific gridded emissions inventory for one year.
- A comprehensive study design and preparation (Mueller, et al., 1977).
- Meteorological regime stratification of sampling schedules to minimize costs while still representing an entire year.
- Characterization of all major source emissions with respect to particle size and chemical composition.
- Time, space, size, and chemical resolution of ambient suspended particulate matter.
- Identification and quantification of major sources by the mass balance receptor model.
- Comparison of mass balance and dispersion model results and adjustments to each.

One of the unique aspects of the PACS was the interaction of the source and receptor models to reinforce each other. The emissions inventory created for the dispersion model was used to identify the most likely sources for emissions characterization. By its estimates of likely ambient concentrations and variability with wind direction, it allowed necessary analytical requirements (detection limits) and sample durations to be estimated. Initially, mass balance calculations did not agree with dispersion model results. An examination of the emissions inventory resulted in corrections and results of the two models did agree within reasonable margins for error (Core, et al., 1982). Control strategy options were outlined which probably would not have been proposed without the results of the PACS. Several of these options are being implemented and it appears that Portland's air quality is improving.

Because of the in-kind donations and development work which went into the PACS, it is difficult to estimate its total cost. Estimates range from $300,000 to $1,000,000. The cost of misplaced controls is agreed to have been much higher than the upper limit of the cost of the study.

6.0 SUMMARY AND CONCLUSIONS

6.1 Summary

It should be apparent from this technical document that, considering the state-of-the-art of receptor and source (dispersion) modeling and composite source apportionment methods, there are no fool-proof step-by-step procedures or recipes for studying particulate matter apportionment and making decisions on the results. Nevertheless, there are a large number of useful tools to assist the air resource manager in carrying out such studies. The selection and application of these tools will depend on:

- Objectives of the study.
- Resources available.
- Technical expertise and innovativeness of the project team.
- Availability and accessibility of data bases.
- Availability of sophisticated sampling and analytical equipment.

Some of the techniques described are well within the resources of even small agencies (e.g., the methods described in Section 2.3.7 - Preliminary or Qualitative Receptor Models) while others require highly trained statisticians and computers of significant size (see Section 2.3.2 - Factor Analysis) and meteorologists with considerable modeling experience (the ISC model described in Section 2.2.2).

It should be clear, however, that in apportioning source contributions in ambient particulate matter studies no single method (e.g., dispersion modeling or a specific receptor model) will ordinarily suffice. Invariably some sort of a composite methodology will be needed.

It has been reasonably well established that most dispersion models when properly applied will predict source impact at a receptor within a factor of two of the correct or measured value. As was pointed out earlier, the mass balance model can apportion generalized source categories within this same range. If one can assume that a dispersion model operating on several sources and a single receptor is a more accurate representation of relative contribution than of total impact, it follows that combining the dispersion and receptor models or two receptor models will produce a much more accurate representation of source contributions than use of each independently. While it is easy for anyone working in this area to believe this statement, the state of technology is such that it is not possible to put error bars on the results of any application of composite methods. Suffice it to say that the results would be better than the use of a single method. The same is true for the combined use of two receptor models.

6.2 Conclusions

An analysis of source contributions to particulate matter levels at one or more receptor locations should start the analysis with elements of the Level I approach (Section 4.3). The air resource specialist responsible for the source apportionment study would need first to become intimately familiar with available data on particulate matter, their trends, the adequacy of the sampling array and the influence of basic meteorological factors as outlined in Section 2.3.7. Furthermore, if an adequate emissions inventory for particulate matter sources did not exist, preparing such an inventory would be a first order of business. The same can be said for the assembly of existing meteorological data.

In progressing to higher levels and more complex and costly approaches, the analysts must carefully weigh the objectives of the analysis and the cost effectiveness of more sophisticated techniques. If the source contribution is needed in only general terms or, more likely, if the sources of nonattainment are relatively straightforward, the techniques of a Level I approach may be adequate. If, on the other hand, specific contributions of selected sources in a complex airshed are needed for control strategy development on a size selective basis, and where emission controls will be costly, a Level II or III approach will be needed. The cost range between Level I and III approaches can vary by more than an order of magnitude (e.g., $10,000 to $500,000).

The application of composite source apportionment techniques is a stepwise, and to some extent, an iterative process where the effectiveness of each added technique is evaluated in terms of increasing the accuracy of the results in relation to the added time and costs.

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APPENDIX A

RESULTS OF SELECTED MODEL VERIFICATION AND EVALUATION STUDIES PERTAINING TO THE 6 ASSUMPTIONS EMPLOYED BY THE MASS BALANCE MODEL

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RESULTS OF SELECTED MODEL VERIFICATION AND EVALUATION STUDIES PERTAINING TO THE 6 ASSUMPTIONS EMPLOYED BY THE MASS BALANCE MODEL

1. Source Composition

Source compositions will vary systematically and randomly. This variability is caused by 1) transformations with transport time between source and receptor (an example is the volatilization of bromine in auto exhaust; e.g., Bowman, et al., 1974), 2) differences in the fuel type or operating processes between similar sources or of the same source in time (an example is the review of lead concentrations in auto exhaust from different automobiles using different fuels by Pierson and Brachaczek, 1976), and 3) uncertainties of the measurement process.

Watson (1979) and Currie, et al., (1983) introduced systematic errors into source compositions to evaluate the effects on source contribution calculations and found:

- The error in the estimated source contributions due to biases (i.e., proportional increases or decreases) in the source compositions is in direct proportion to the magnitude of that bias (Watson, 1979).

- For random errors associated with estimates of average source compositions, the magnitude of the source contribution errors decreases as the number of components increases (Watson, 1979).

- In comparing a number of mass balance solutions on simulated data in which random errors and biases were introduced to the source compositions, Currie, et al., (1983) found "Only the effective variance [solution] explicitly included the effect of source profile uncertainties, but these were treated as random rather than as systematic error components."

2. Components Add Linearly

No studies have been performed to evaluate deviations from this assumption. While the deviations from this assumption are generally considered to be small, the conversion of gases to particles and reactions between particles are not inherently linear processes (e.g., Friedlander, 1977).

3. All Sources Have Been Identified

Watson (1979) systematically increased the number of sources contributing to his simulated data from 4 to 8 contributors while solving the mass balance equations assuming only four sources. He also examined the case of including more sources in the least squares solution than those which actually contribute. The results were:

- Underestimating the number of sources has little effect on the calculated source contributions if the prominant properties contributed by the source are excluded from the solution.
- When the number of sources is underestimated and when prominent properties of the omitted sources are included in the calculation of source contributions, the contributions of sources with properties in common with the omitted sources are overestimated.
- When source types which are actually present are excluded from the effective variance least squares solution, ratios of calculated to measured concentrations are often outside of the 0.5 to 2.0 range, and the sum of the source contributions is much less than the total measured mass. The low calculated/measured ratios indicate which source compositions should be included.
- When the number of sources is overestimated, the sources which are not actually present yield contributions less than their precisions if their properties are significantly distinct from other sources. The over-specification of sources decreases the precisions of the true source contribution estimates.

4. Number of Sources Less Than Number of Components

It is likely that the number of individual sources contributing to receptor concentrations is much larger than the number of properties which can be measured. It is therefore necessary to group sources into source types of similar compositions such that this assumption is met. For most commonly measured aerosol properties, meeting Assumption 5 practically defines these groupings. Henry (1977) speculates that the linear programming solution might work if the number of sources is greater than the number of components, but he offers no proof. None of the least squares solutions will work if this assumption is not met.

5. Compositions are Linearly Independent

Watson (1979) examined effects of deviations from this assumption with simulated data while Gordon, et al., (1981) studied it with ambient measurements. Henry (1982) has devised an analytical method of determining the degree of linear dependence in typical mass balance applications for which only a few tests are available. His algorithm could be incorporated into the routine mass balance model to identify linear independence at given precision levels for all combinations of sources and components. The results of these studies show:

- With most commonly measured components (i.e., ions, elements, and carbon) and source types (e.g., motor vehicle, crustal, residual oil, sea salt, steel production, wood burning, and various industrial processes), from five to seven sources are linearly independent of each other. Some of the source compositions used in the solution may be better expressed as linear combinations of measured source compositions (Henry, 1982).
- Henry (1982) determined the modified source compositions which would give the same results as a ridge regression solution and noted that: "The apparent ability of ridge regression to solve the multicollinearity problem is seen to be based on implicitly changing the [mass balance] problem to one which is not physically meaningful."

- Gordon, et al., (1981) found instabilities in the ordinary weighted least squares solutions when they removed elemental concentrations which were known to be unique to certain source types. Using simulated data with known perturbations of 0 percent to 20 percent, Watson (1979) found: "In the presence of likely uncertainties, sources such as urban dust and continental background dust cannot be adequately resolved by least squares fitting, even though their compositions are not identical. Several nearly unique ratios must exist for good separation.

6. Measurement Errors Random and Uncorrelated

These least squares solutions methods are derived from maximum likelihood theory which requires this assumption. In reality, we know very little about the distribution of errors for the source compositions and the ambient concentrations. For small errors (i.e. <10 percent) the actual distribution may not be important, but for large errors it probably is; a symmetric distribution becomes less probable as the coefficient of variation of the measurement increases. Though evaluation of deviation from this assumption could be undertaken by generating simulated data perturbed by random numbers drawn from lognormal, uniform, and other distributions, these tests have never been performed.

APPENDIX B

SOURCE COMPOSITION REFERENCES

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